

Dicyclohexyl
phthalate C20H26O4
structure

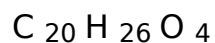


**ASSIGN
BUSTER**

Contents

- Retention Index (Linear):

Molecular



Formula

Average mass 330. 418 Da

Density 1. 1±0. 1 g/cm³Boiling Point 425. 8±18. 0 °C at
760 mmHg

Flash Point 206. 6±19. 6 °C

Molar

$$91. 2\pm 0. 4 \text{ cm}^3$$

Refractivity

Polarizability 36. 1±0. 5 10⁻²⁴
cm³

Surface

$$45. 8\pm 5. 0 \text{ dyne/cm}$$

Tension

Molar Volume 288. 6±5. 0 cm³

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Predicted - Mcule
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

65 °C
TCIP0293

62-64 °C
Merck

Millipore1191, 800920

66 °C
Jean-Claude

Bradley Open Melting

Point Dataset21072

63-67 °C
Alfa

AesarH56004

63-67 °C

(Literature)LabNetwork

LN00223414

- **Experimental Boiling Point:**

200-235 °C / 4 mmHg

(426. 6939-476. 9317

°C / 760

mmHg)LabNetworkLN0

0223414

- **Experimental Flash Point:**

207

°CLabNetworkLN00223414

- **Experimental Gravity:**

1. 383 g/mLAlfa

AesarH56004

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

65 °CTCI

65

°CTCIP0293

- Miscellaneous

- **Safety:**

26-37-60Alfa

AesarH56004

36/37/38Alfa

AesarH56004

GHS07BiosynthW-

104111

H315; H319;

H335BiosynthW-

104111

H315-H319-H335Alfa

AesarH56004

IrritantSynQuest2623-

1-58

P261;

P305+P351+P338Biosy

nthW-104111

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarH56004

WarningAlfa

AesarH56004

WarningBiosynthW-

104111

- Gas Chromatography

- **Retention Index (Kovats):**

2561 (estimated with

error: 47)NIST

Spectramainlib_250710

, replib_232967,

replib_313012,

replib_315339

2453 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column length: 1. 5 m;

Column type: Packed;

CAS no: 84617; Active

phase: SE-30; Carrier

gas: He; Substrate:

Chromosorb G HP (80-

100 mesh); Data type:

Kovats RI; Authors:

Ramsey, J. D.; Lee, T.

D.; Osselton, M. D.;

Moffat, A. C., Gas-liquid

chromatographic

retention indices of 296

non-drug substances

on SE-30 or OV-1 likely

to be encountered in

toxicological analyses,
J. Chromatogr., 184,
1980, 185-206.)NIST
Spectranist ri

2461 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 1. 5 m;
Column type: Packed;
CAS no: 84617; Active
phase: SE-30; Carrier
gas: He; Substrate:
Chromosorb G HP (80-
100 mesh); Data type:
Kovats RI; Authors:
Ramsey, J. D.; Lee, T.
D.; Osselton, M. D.;
Moffat, A. C., Gas-liquid
chromatographic
retention indices of 296
non-drug substances
on SE-30 or OV-1 likely
to be encountered in
toxicological analyses,

J. Chromatogr., 184,
1980, 185-206.)NIST

Spectranist ri

2475 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0.3

mm; Column length: 50

m; Column type:

Capillary; Start T: 250

C; CAS no: 84617;

Active phase: SE-30;

Carrier gas: He; Phase

thickness: 0.39 um;

Data type: Kovats RI;

Authors: Friocourt, M.

P.; Berthou, F.; Picart,

D.; Dreano, Y.; Floch,

H. H., Glass Capillary

Column Gas

Chromatography of

Phthalate Esters, J.

Chromatogr., 172,

1979, 261-271.)NIST

Spectranist ri

- **Retention Index (Normal Alkane):**

2434 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0.32

mm; Column length: 25

m; Column type:

Capillary; Heat rate: 3

K/min; Start T: 80 C;

End T: 260 C; CAS no:

84617; Active phase:

Ultra-1; Carrier gas:

He; Phase thickness: 0.

25 um; Data type:

Normal alkane RI;

Authors: Okumura, T.,

retention indices of

environmental

chemicals on methyl

silicone capillary

column, Journal of

Environmental

Chemistry (Japan),

1(2), 1991, 333-

358.)NIST Spectranist ri

2454. 2 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column length: 1. 1 m;

Column type: Packed;

Heat rate: 8. 5 K/min;

Start T: 50 C; End T:

300 C; CAS no: 84617;

Active phase: OV-101;

Carrier gas: N2;

Substrate: Chromosorb

W HP; Data type:

Normal alkane RI;

Authors: Saxton, W. L.,

Emergence

temperature indices

and relative retention

times of pesticides and

industrial chemicals

determined by linear

programmed

temperature gas

chromatography, J.
Chromatogr., 393,
1987, 175-194.)NIST
Spectranist ri

2453 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Other;
CAS no: 84617; Active
phase: Methyl Silicone;
Data type: Normal
alkane RI; Authors:
Ardrey, R. E.; Moffat, A.
C., Gas-liquid
chromatographic
retention indices of
1318 substances of
toxicological interest
on SE-30 or OV-1
stationary phase, J.
Chromatogr., 220,
1981, 195-252.)NIST
Spectranist ri

2461 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Other;
CAS no: 84617; Active
phase: Methyl Silicone;
Data type: Normal
alkane RI; Authors:
Ardrey, R. E.; Moffat, A.
C., Gas-liquid
chromatographic
retention indices of
1318 substances of
toxicological interest
on SE-30 or OV-1
stationary phase, J.
Chromatogr., 220,
1981, 195-252.)NIST
Spectranist ri

2483. 8 (Program type:
Complex; Column...
(show more)class:
Semi-standard non-
polar; Column

diameter: 0. 25 mm;
Column length: 30 m;
Column type: Capillary;
Description: 80C(1min)
=> 50C/min => 200C
=> 15C/min => 350C
(2min); CAS no: 84617;
Active phase: DB-5MS;
Phase thickness: 0. 25
um; Data type: Normal
alkane RI; Authors:
George, C.; Prest, H., A
new approach to the
analysis of phthalate
esters by GC/MS,
2003.)NIST Spectranist
ri

2511. 3 (Program type:
Complex; Column...
(show more)class:
Semi-standard non-
polar; Column
diameter: 0. 2 mm;
Column length: 25 m;
Column type: Capillary;

Description:

100C(1min) =>

30C/min=>

150C(2min) =>

3C/min=> 205C =>

10C/min =>

260C(29min); CAS no:

84617; Active phase:

SE-54; Phase thickness:

0.33 um; Data type:

Normal alkane RI;

Authors: Stan, H.-J.,

Pesticide residue

analysis in foodstuffs

applying capillary gas

chromatography with

mass spectrometric

detection State-of-the-

art use of modified

DFG-multimethod S19

and automated data

evaluation, J.

Chromatogr. A, 892,

2000, 347-377.)NIST

Spectranist ri

2468 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column diameter: 0.25
mm; Column length: 30
m; Column type:
Capillary; Heat rate: 15
K/min; Start T: 120 C;
End T: 160 C; End time:
16 min; CAS no: 84617;
Active phase: DB-5;
Data type: Normal
alkane RI; Authors:
Lopez-Avila, V.;
Milanes, J.; Beckert, W.
F., Single-laboratory
evaluation of method
8060 for the
determination of
phthalates in
environmental
samples, J. Ass. Offic.
Anal. Chem, 74(5),
1991, 793-808.)NIST
Spectranist ri

2516. 1 (Program type:
Complex; Column...
(show more)class:
Semi-standard non-
polar; Column
diameter: 0. 53 mm;
Column length: 30 m;
Column type: Capillary;
Description: 150 0C (0.
5 min) ^ 3 0C/min ->
220 0C ^ 5 0C/min ->
275 0C (15 min); CAS
no: 84617; Active
phase: DB-5; Data
type: Normal alkane RI;
Authors: Lopez-Avila,
V.; Milanes, J.; Beckert,
W. F., Single-laboratory
evaluation of method
8060 for the
determination of
phthalates in
environmental
samples, J. Ass. Offic.
Anal. Chem, 74(5),
1991, 793-808.)NIST

Spectranist ri

- **Retention Index (Linear):**

2472 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column type: Packed;

Heat rate: 10 K/min;

Start T: 100 C; End T:

340 C; CAS no: 84617;

Active phase: SE-30;

Carrier gas: N2;

Substrate: Chromosorb

Q; Data type: Linear RI;

Authors: Messadi, D.;

Vergnaud, J.-M., Quick

identification and

analysis of plasticizers

in PVC by programmed-

temperature gas

chromatography using

the best stationary

phases, J. Appl. Polym.

Sci., 24, 1979, 1215-

1225.)NIST Spectranist

ri

Predicted data is generated using the ACD/Labs Percepta Platform -
PhysChem Module

Density:	1.1 ± 0.1 g/cm ³
Boiling Point:	425.8 ± 18.0 °C at 760 mmHg
Vapour Pressure:	0.0 ± 1.0 mmHg at 25°C
Enthalpy of Vaporization:	68.0 ± 3.0 kJ/mol
Flash Point:	206.6 ± 19.6 °C
Index of Refraction:	1.544
Molar Refractivity:	91.2 ± 0.4 cm ³
#H bond acceptors:	4
#H bond donors:	0
#Freely Rotating Bonds:	6
#Rule of 5 Violations:	1
ACD/LogP:	5.76
ACD/LogD (pH 5.5):	5.32

ACD/BCF (pH 5. 5):	6482. 34
ACD/KOC (pH 5. 5):	18622. 12
ACD/LogD (pH 7. 4):	5. 32
ACD/BCF (pH 7. 4):	6482. 34
ACD/KOC (pH 7. 4):	18622. 12
Polar Surface Area:	53 Å ²
Polarizability:	36. 1±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	45. 8±5. 0 dyne/cm
Molar Volume:	288. 6±5. 0 cm ³

Predicted data is generated using the US Environmental Protection Agency's

EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 6. 20Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 394. 85 (Adapted Stein & Brown method)Melting Pt (deg C): 61. 45 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 58E-006 (Modified Grain method)MP (exp database): 66 deg CBP (exp database): 218 @ 4. 5 mm Hg deg CVP (exp database): 8. 69E-07 mm Hg at 25 deg CSubcooled liquid VP: 2. 21E-006 mm Hg (25 deg C, exp database VP)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 04098log Kow used: 6. 20 (estimated)no-melting pt equation usedWater Sol (Exper. database match) = 4 mg/L (24 deg C)Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2. 4027 mg/LWat Sol (Exper. database match) = 4. 00Exper. Ref: YALKOWSKY, SH & DANNENFELSER, RM (1992)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: EstersHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 39E-007 atm-m3/moleGroup Method: 6. 43E-008 atm-m3/moleExper Database: 1. 00E-07 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 859E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 6. 20 (KowWin est)Log Kaw used: -5. 388 (exp database)Log Koa (KOAWIN v1. 10 estimate): 11. 588Log Koa (experimental database):

<https://assignbuster.com/dicyclohexyl-phthalate-c20h26o4-structure/>

NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9386Biowin2 (Non-Linear Model) : 0. 9985Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7494 (weeks-months)Biowin4 (Primary Survey Model) : 3. 8289 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6716Biowin6 (MITI Non-Linear Model): 0. 6144Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3232Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 000295 Pa (2. 21E-006 mm Hg)Log Koa (Koawin est): 11. 588Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 0102 Octanol/air (Koa) model: 0. 0951 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 269 Mackay model : 0. 449 Octanol/air (Koa) model: 0. 884 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 2718 E-12 cm3/molecule-secHalf-Life = 0. 441 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 288 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 359 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 764E+004Log Koc: 4. 246 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 1. 883E-002 L/mol-secKb Half-Life at pH 8: 1. 166 years Kb Half-Life at pH 7: 11. 662 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 4. 076 (BCF = 1. 191e+004)log Kow used: 6. 20 (estimated)Volatilization from Water: Henry LC: 1E-007 atm-m3/mole (Henry experimental database)Half-Life from Model River: 1. 064E+004 hours (443. 5 days)Half-Life from Model Lake : 1. 163E+005 hours (4845 days)Removal In Wastewater Treatment: Total removal: 92. 84 percentTotal biodegradation: 0. 77 percentTotal sludge adsorption: 92. 07 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 113 10. 6 1000 Water 3. 16 900 1000 Soil 37 1. 8e+003 1000 Sediment 59. 7 8. 1e+003 0 Persistence Time: 2. 88e+003 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop