

Bromothymol blue
c₂₇h₂₈br₂o₅s
structure



**ASSIGN
BUSTER**

Contents

- Safety:

Molecular C₂₇ H₂₈ Br

Formula 2 O₅ S

Average 624. 381

mass Da

Density 1. 5±0. 1

g/cm³

Boiling 614. 3±55.

Point 0 °C at 760

mmHg

Flash Point 325. 3±31.

5 °C

Molar 144. 8±0.

Refractivity 4 cm³

Polarizabilit 57. 4±0. 5

y 10⁻²⁴ cm³

Surface 54. 1±3. 0

Tension dyne/cm

Molar 404. 9±3.

Volume 0 cm³

- Experimental data
- Predicted – ACD/Labs
- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

200-202

°CAIfa Aesar

200

°COxford

University

Chemical

Safety Data

(No longer

updated)Mo

re details

200-202

°CAIfa

AesarA1774

6

200 °CJean-

Claude

Bradley

Open

Melting

Point

Dataset154

10

201 °CJean-

Claude

Bradley

Open

Melting

Point

Dataset212

38, 6586

- **Experimental Boiling Point:**

184. 9 °CBiosynthJ-

610060

- **Experimental Gravity:**

63 g/mL BiosynthJ-

610060

- Miscellaneous

- **Appearance:**

purple to

pink

powderOxfo

rd

University

Chemical

Safety Data

(No longer

updated)Mo

re details

- **Stability:**

Stable.

Incompatibl

e with

strong

oxidizing

agents.

Oxford

University

Chemical

Safety Data

(No longer

updated)Mo

re details

- **Safety:**

CAUTION:

May irritate

skin and

eyesAlfa

AesarA1774

6

Safety

glasses.

Oxford

University

Chemical

Safety Data

(No longer

updated)Mo

re details

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

Density: $1.5 \pm 0.1 \text{ g/cm}^3$

Boiling Point: $614.3 \pm 55.0 \text{ }^\circ\text{C}$ at 760 mmHg

Vapour Pressure: $0.0 \pm 1.8 \text{ mmHg}$ at 25°C

<https://assignbuster.com/bromothymol-blue-c27h28br2o5s-structure/>

Enthalpy of Vaporization:	94. 5±3. 0 kJ/mol
Flash Point:	325. 3±31. 5 °C
Index of Refraction:	1. 634
Molar Refractivity:	144. 8±0. 4 cm ³
#H bond acceptors:	5
#H bond donors:	2
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	2
ACD/LogP:	8. 60
ACD/LogD (pH 5. 5):	7. 90
ACD/BCF (pH 5. 5):	575174. 94
ACD/KOC (pH 5. 5):	440905. 75
ACD/LogD (pH 7. 4):	6. 27
ACD/BCF (pH 7. 4):	13411. 26
ACD/KOC (pH 7. 4):	10280. 53

Polar Surface Area:	92 Å ²
Polarizability:	57.4 ± 0.5 10 ⁻²⁴ cm ³
Surface Tension:	54.1 ± 3.0 dyne/cm
Molar Volume:	404.9 ± 3.0 cm ³

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop