

# [Bromothymol blue c27h28br2o5s structure](https://assignbuster.com/bromothymol-blue-c27h28br2o5s-structure/)

Contents

* Safety:

|  |  |
| --- | --- |
| Molecular Formula  | C 27 H 28 Br 2 O 5 S  |
| Average mass  | 624. 381 Da  |
| Density  | 1. 5±0. 1 g/cm 3  |
| Boiling Point  | 614. 3±55. 0 °C at 760 mmHg  |
| Flash Point  | 325. 3±31. 5 °C  |
| Molar Refractivity  | 144. 8±0. 4 cm 3  |
| 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  |

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

## Experimental Melting Point:

|  |
| --- |
| 200-202 °CAlfa Aesar  |
| 200 °COxford University Chemical Safety Data (No longer updated)More details  |
| 200-202 °CAlfa AesarA17746  |
| 200 °CJean-Claude Bradley Open Melting Point Dataset15410  |
| 201 °CJean-Claude Bradley Open Melting Point Dataset21238, 6586  |

## Experimental Boiling Point:

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| --- |
| 184. 9 °CBiosynthJ-610060  |

## Experimental Gravity:

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| --- |
| 63 g/mLBiosynthJ-610060  |

* Miscellaneous

## Appearance:

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| purple to pink powderOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

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| Stable. Incompatible with strong oxidizing agents. Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

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| --- |
| CAUTION: May irritate skin and eyesAlfa AesarA17746  |
| Safety glasses. Oxford University Chemical Safety Data (No longer updated)More details  |

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

|  |  |
| --- | --- |
| Density:  | 1. 5±0. 1 g/cm 3  |
| Boiling Point:  | 614. 3±55. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±1. 8 mmHg at 25°C  |
| 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