

# [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| 200 °COxford University Chemical Safety Data (No longer updated)More details |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:

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| purple to pink powderOxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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 Oxford University Chemical Safety Data (No longer updated)More details |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

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| --- | --- |
| 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 |

|  |  |
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| 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