# 2-Hydroxy-5-nitrobenzyl bromide

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|---|---|
| **Other names:** | «alpha»-Bromo-4-nitro-o-cresol |
| | Phenol, 2-(bromomethyl)-4-nitro- |
| | o-Cresol, «alpha»-bromo-4-nitro- |
| | Alpha-bromo-4-nitro-O-cresol |
| **Inchi:** | InChI=1S/C7H6BrNO3/c8-4-5-3-6(9(11)12)1-2-7(5)10/h1-3,10H,4H2 |
| **InchiKey:** | KFDPCYZHENQOBV-UHFFFAOYSA-N |
| **Formula:** | C7H6BrNO3 |
| **SMILES:** | O=[N+]([O-])c1ccc(O)c(CBr)c1 |
| **Mol. weight [g/mol]:** | 232.03 |
| **CAS:** | 772-33-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 6.09 | kJ/mol | Joback Method |
| hf | -124.49 | kJ/mol | Joback Method |
| hfus | 29.97 | kJ/mol | Joback Method |
| hvap | 70.15 | kJ/mol | Joback Method |
| log10ws | -2.98 | | Crippen Method |
| logp | 2.195 | | Crippen Method |
| mcvol | 126.520 | ml/mol | McGowan Method |
| pc | 5536.07 | kPa | Joback Method |
| tb | 689.84 | K | Joback Method |
| tc | 961.43 | K | Joback Method |
| tf | 522.72 | K | Joback Method |
| vc | 0.429 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 288.25 | J/mol×K | 689.84 | Joback Method |
| cpg | 296.48 | J/mol×K | 735.10 | Joback Method |
| cpg | 304.08 | J/mol×K | 780.37 | Joback Method |
| cpg | 311.18 | J/mol×K | 825.63 | Joback Method |
| cpg | 317.94 | J/mol×K | 870.90 | Joback Method |

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|---|---|---|---|---|
| cpg | 324.51 | J/mol×K | 916.16 | Joback Method |
| cpg | 331.01 | J/mol×K | 961.43 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C772338&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |