

Benzamide, 2-bromo-N-pentyl-

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H16BrNO/c1-2-3-6-9-14-12(15)10-7-4-5-8-11(10)13/h4-5,7-8H,2-3,6,9H2,1 |
| InchiKey: | RCKFKZXUGXJCQK-UHFFFAOYSA-N |
| Formula: | C12H16BrNO |
| SMILES: | CCCCCN=C(O)c1ccccc1Br |
| Mol. weight [g/mol]: | 270.17 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -119.42 | kJ/mol | Joback Method |
| hvap | 71.75 | kJ/mol | Joback Method |
| log10ws | -4.20 | | Crippen Method |
| logp | 3.944 | | Crippen Method |
| mcvol | 185.230 | ml/mol | McGowan Method |
| pc | 2517.59 | kPa | Joback Method |
| rinsol | 2017.00 | | NIST Webbook |
| rinsol | 2017.00 | | NIST Webbook |
| tb | 740.52 | K | Joback Method |
| tc | 956.69 | K | Joback Method |

Sources

| | |
|------------------------|---|
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407116&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|--------------|---|
| hf: | Enthalpy of formation 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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |

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