

Benzamide, 3-bromo-N-butyl-N-2-ethylhexyl-

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| Inchi: | InChI=1S/C19H30BrNO/c1-4-7-10-16(6-3)15-21(13-8-5-2)19(22)17-11-9-12-18(20)14-17 |
| InchiKey: | HASZMZNMWDDDDAS-UHFFFAOYSA-N |
| Formula: | C19H30BrNO |
| SMILES: | CCCCC(CC)CN(CCCC)C(=O)c1cccc(Br)c1 |
| Mol. weight [g/mol]: | 368.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 205.62 | kJ/mol | Joback Method |
| hf | -234.43 | kJ/mol | Joback Method |
| hfus | 45.00 | kJ/mol | Joback Method |
| hvap | 75.66 | kJ/mol | Joback Method |
| log10ws | -6.72 | | Crippen Method |
| logp | 5.908 | | Crippen Method |
| mcvol | 283.860 | ml/mol | McGowan Method |
| pc | 1493.04 | kPa | Joback Method |
| rinpola | 2933.00 | | NIST Webbook |
| rinpola | 2933.00 | | NIST Webbook |
| tb | 797.81 | K | Joback Method |
| tc | 1001.82 | K | Joback Method |
| tf | 470.03 | K | Joback Method |
| vc | 1.071 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 827.31 | J/molxK | 797.81 | Joback Method |
| cpg | 844.36 | J/molxK | 831.81 | Joback Method |
| cpg | 860.37 | J/molxK | 865.81 | Joback Method |
| cpg | 875.40 | J/molxK | 899.82 | Joback Method |
| cpg | 889.52 | J/molxK | 933.82 | Joback Method |
| cpg | 902.80 | J/molxK | 967.82 | Joback Method |
| cpg | 915.30 | J/molxK | 1001.82 | 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=U415665&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |

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 |
| rinpola: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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