

Benzamide, 4-methyl-N-butyl-N-octyl-

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C20H33NO/c1-4-6-8-9-10-11-17-21(16-7-5-2)20(22)19-14-12-18(3)13-15-19/h |
| InchiKey: | LEEZXKADHGANNK-UHFFFAOYSA-N |
| Formula: | C20H33NO |
| SMILES: | CCCCCCCCN(CCCC)C(=O)c1ccc(C)cc1 |
| Mol. weight [g/mol]: | 303.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 202.16 | kJ/mol | Joback Method |
| hf | -276.12 | kJ/mol | Joback Method |
| hfus | 45.83 | kJ/mol | Joback Method |
| hvap | 71.84 | kJ/mol | Joback Method |
| log10ws | -6.28 | | Crippen Method |
| logp | 5.598 | | Crippen Method |
| mvol | 280.450 | ml/mol | McGowan Method |
| pc | 1311.80 | kPa | Joback Method |
| rinpol | 2999.00 | | NIST Webbook |
| rinpol | 2999.00 | | NIST Webbook |
| tb | 754.97 | K | Joback Method |
| tc | 945.36 | K | Joback Method |
| tf | 436.50 | K | Joback Method |
| vc | 1.071 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 837.43 | J/molxK | 754.97 | Joback Method |
| cpg | 856.07 | J/molxK | 786.70 | Joback Method |
| cpg | 873.65 | J/molxK | 818.43 | Joback Method |
| cpg | 890.24 | J/molxK | 850.16 | Joback Method |
| cpg | 905.89 | J/molxK | 881.89 | Joback Method |
| cpg | 920.64 | J/molxK | 913.63 | Joback Method |
| cpg | 934.54 | J/molxK | 945.36 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U415926&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/87-606-3/Benzamide-4-methyl-N-butyl-N-octyl.pdf>

Generated by Cheméo on 2025-02-08 18:25:25.290239424 +0000 UTC m=+2247341.137165055.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.