# Benzamide, 2,5-di(trifluoromethyl)-N-hept-2-yl-

**Inchi:** InChI=1S/C16H19F6NO/c1-3-4-5-6-10(2)23-14(24)12-9-11(15(17,18)19)7-8-13(12)16(20
**InchiKey:** RUBWLEAJYADTRH-UHFFFAOYSA-N
**Formula:** C16H19F6NO
**SMILES:** CCCCCC(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
**Mol. weight [g/mol]:** 355.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1028.16 | kJ/mol | Joback Method |
| hf | -1418.53 | kJ/mol | Joback Method |
| hfus | 37.29 | kJ/mol | Joback Method |
| hvap | 60.11 | kJ/mol | Joback Method |
| log10ws | -6.65 | | Crippen Method |
| logp | 5.423 | | Crippen Method |
| mcvol | 234.710 | ml/mol | McGowan Method |
| pc | 1478.15 | kPa | Joback Method |
| rinpol | 1652.00 | | NIST Webbook |
| rinpol | 1652.00 | | NIST Webbook |
| tb | 694.88 | K | Joback Method |
| tc | 873.94 | K | Joback Method |
| tf | 417.51 | K | Joback Method |
| vc | 0.945 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 681.40 | J/mol×K | 694.88 | Joback Method |
| cpg | 695.60 | J/mol×K | 724.72 | Joback Method |
| cpg | 708.93 | J/mol×K | 754.57 | Joback Method |
| cpg | 721.42 | J/mol×K | 784.41 | Joback Method |
| cpg | 733.15 | J/mol×K | 814.26 | Joback Method |
| cpg | 744.15 | J/mol×K | 844.10 | Joback Method |
| cpg | 754.48 | J/mol×K | 873.94 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407921&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

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