# Benzamide, 4-(trifluoromethyl)-N-2-ethylhexyl-

**Inchi:** InChI=1S/C16H22F3NO/c1-3-5-6-12(4-2)11-20-15(21)13-7-9-14(10-8-13)16(17,18)19/h7
**InchiKey:** HNJDQUWAOKLFTP-UHFFFAOYSA-N
**Formula:** C16H22F3NO
**SMILES:** CCCCC(CC)CNC(=O)c1ccc(C(F)(F)F)cc1
**Mol. weight [g/mol]:** 301.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -436.94 | kJ/mol | Joback Method |
| hf | -809.98 | kJ/mol | Joback Method |
| hfus | 35.85 | kJ/mol | Joback Method |
| hvap | 63.20 | kJ/mol | Joback Method |
| log10ws | -5.61 | | Crippen Method |
| logp | 4.652 | | Crippen Method |
| mcvol | 229.400 | ml/mol | McGowan Method |
| pc | 1639.10 | kPa | Joback Method |
| rinpol | 1915.00 | | NIST Webbook |
| rinpol | 1915.00 | | NIST Webbook |
| tb | 695.32 | K | Joback Method |
| tc | 884.23 | K | Joback Method |
| tf | 400.80 | K | Joback Method |
| vc | 0.901 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 655.79 | J/mol×K | 695.32 | Joback Method |
| cpg | 671.38 | J/mol×K | 726.81 | Joback Method |
| cpg | 686.02 | J/mol×K | 758.29 | Joback Method |
| cpg | 699.77 | J/mol×K | 789.78 | Joback Method |
| cpg | 712.67 | J/mol×K | 821.26 | Joback Method |
| cpg | 724.78 | J/mol×K | 852.75 | Joback Method |
| cpg | 736.14 | J/mol×K | 884.23 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407302&Units=SI |

# 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 |
| **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 |