# Benzamide, 3-trifluoromethyl-N-ethyl-N-propyl-

**Inchi:** InChI=1S/C13H16F3NO/c1-3-8-17(4-2)12(18)10-6-5-7-11(9-10)13(14,15)16/h5-7,9H,3-4

**InchiKey:** LWVMRQVYLJIFOQ-UHFFFAOYSA-N

**Formula:** C13H16F3NO

**SMILES:** CCCN(CC)C(=O)c1cccc(C(F)(F)F)c1

**Mol. weight [g/mol]:** 259.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -438.37 | kJ/mol | Joback Method |
| hf | -728.72 | kJ/mol | Joback Method |
| hfus | 29.52 | kJ/mol | Joback Method |
| hvap | 52.51 | kJ/mol | Joback Method |
| log10ws | -3.97 | | Crippen Method |
| logp | 3.578 | | Crippen Method |
| mcvol | 187.130 | ml/mol | McGowan Method |
| pc | 2056.76 | kPa | Joback Method |
| rinpol | 2706.00 | | NIST Webbook |
| rinpol | 2706.00 | | NIST Webbook |
| tb | 589.39 | K | Joback Method |
| tc | 776.96 | K | Joback Method |
| tf | 361.80 | K | Joback Method |
| vc | 0.723 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 481.18 | J/mol×K | 589.39 | Joback Method |
| cpg | 496.18 | J/mol×K | 620.65 | Joback Method |
| cpg | 510.25 | J/mol×K | 651.91 | Joback Method |
| cpg | 523.44 | J/mol×K | 683.18 | Joback Method |
| cpg | 535.79 | J/mol×K | 714.44 | Joback Method |
| cpg | 547.35 | J/mol×K | 745.70 | Joback Method |
| cpg | 558.17 | J/mol×K | 776.96 | Joback Method |

# Sources

| | |
|---|---|
| **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=U415568&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |