# Benzamide, 2,3,4-trifluoro-N-(hept-2-yl)-

**Inchi:** InChI=1S/C14H18F3NO/c1-3-4-5-6-9(2)18-14(19)10-7-8-11(15)13(17)12(10)16/h7-9H,3-
**InchiKey:** RVRDVFRBRFJVEY-UHFFFAOYSA-N
**Formula:** C14H18F3NO
**SMILES:** CCCCCC(C)NC(=O)c1ccc(F)c(F)c1F
**Mol. weight [g/mol]:** 273.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -475.88 | kJ/mol | Joback Method |
| hf | -782.89 | kJ/mol | Joback Method |
| hfus | 37.30 | kJ/mol | Joback Method |
| hvap | 61.36 | kJ/mol | Joback Method |
| log10ws | -5.43 | | Crippen Method |
| logp | 3.803 | | Crippen Method |
| mcvol | 201.220 | ml/mol | McGowan Method |
| pc | 1846.75 | kPa | Joback Method |
| rinpol | 1709.00 | | NIST Webbook |
| rinpol | 1709.00 | | NIST Webbook |
| tb | 662.75 | K | Joback Method |
| tc | 848.05 | K | Joback Method |
| tf | 400.88 | K | Joback Method |
| vc | 0.800 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 545.12 | J/mol×K | 662.75 | Joback Method |
| cpg | 559.18 | J/mol×K | 693.63 | Joback Method |
| cpg | 572.49 | J/mol×K | 724.52 | Joback Method |
| cpg | 585.07 | J/mol×K | 755.40 | Joback Method |
| cpg | 596.94 | J/mol×K | 786.28 | Joback Method |
| cpg | 608.14 | J/mol×K | 817.17 | Joback Method |
| cpg | 618.67 | J/mol×K | 848.05 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U407263&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 |