# 2,2,3,3,4,4,4-Heptafluoro-N-[2-(2,2,3,3,4,4,4-heptaf

**Inchi:** InChI=1S/C14H6F14N2O2/c15-9(16,11(19,20)13(23,24)25)7(31)29-5-3-1-2-4-6(5)30-8(3
**InchiKey:** FCRWLNOWNDZUEN-UHFFFAOYSA-N
**Formula:** C14H6F14N2O2
**SMILES:** O=C(Nc1ccccc1NC(=O)C(F)(F)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F
**Mol. weight [g/mol]:** 500.19

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2619.58 | kJ/mol | Joback Method |
| hf | -3023.49 | kJ/mol | Joback Method |
| hfus | 37.70 | kJ/mol | Joback Method |
| hvap | 56.85 | kJ/mol | Joback Method |
| log10ws | -6.13 | | Crippen Method |
| logp | 5.229 | | Crippen Method |
| mcvol | 232.240 | ml/mol | McGowan Method |
| pc | 1467.98 | kPa | Joback Method |
| rinpol | 1467.00 | | NIST Webbook |
| rinpol | 1467.00 | | NIST Webbook |
| tb | 729.86 | K | Joback Method |
| tc | 902.60 | K | Joback Method |
| tf | 514.44 | K | Joback Method |
| vc | 0.980 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 718.39 | J/mol×K | 729.86 | Joback Method |
| cpg | 727.41 | J/mol×K | 758.65 | Joback Method |
| cpg | 735.60 | J/mol×K | 787.44 | Joback Method |
| cpg | 743.05 | J/mol×K | 816.23 | Joback Method |
| cpg | 749.87 | J/mol×K | 845.02 | Joback Method |
| cpg | 756.14 | J/mol×K | 873.81 | Joback Method |
| cpg | 761.97 | J/mol×K | 902.60 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373044&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 |

# 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 |