# Methylenedioxyamphetamine, N-heptafluorobutyryl deriv.

**Other names:** MDA, HFB

Butanamide, N-[2-(1,3-benzodioxol-5-yl)-1-methylethyl]-2,2,3,3,4,4,4-heptafluoro-

**Inchi:** InChI=1S/C14H12F7NO3/c1-7(4-8-2-3-9-10(5-8)25-6-24-9)22-11(23)12(15,16)13(17,18)

**InchiKey:** HIHQJXYXAUVMOH-UHFFFAOYSA-N

**Formula:** C14H12F7NO3

**SMILES:** CC(Cc1ccc2c(c1)OCO2)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

**Mol. weight [g/mol]:** 375.24

**CAS:** 156572-19-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1340.75 | kJ/mol | Joback Method |
| hf | -1752.97 | kJ/mol | Joback Method |
| hfus | 40.79 | kJ/mol | Joback Method |
| hvap | 62.79 | kJ/mol | Joback Method |
| log10ws | -4.95 | | Crippen Method |
| logp | 3.295 | | Crippen Method |
| mcvol | 209.180 | ml/mol | McGowan Method |
| pc | 1906.90 | kPa | Joback Method |
| tb | 710.47 | K | Joback Method |
| tc | 901.99 | K | Joback Method |
| tf | 473.30 | K | Joback Method |
| vc | 0.840 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 628.94 | J/mol×K | 710.47 | Joback Method |
| cpg | 640.51 | J/mol×K | 742.39 | Joback Method |
| cpg | 651.18 | J/mol×K | 774.31 | Joback Method |
| cpg | 661.05 | J/mol×K | 806.23 | Joback Method |
| cpg | 670.22 | J/mol×K | 838.15 | Joback Method |
| cpg | 678.79 | J/mol×K | 870.07 | Joback Method |
| cpg | 686.85 | J/mol×K | 901.99 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C156572199&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

| | |
|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |