# Carbonic acid, monoamide, N-(3-methylbutyl)-, octyl ester

**Inchi:** InChI=1S/C14H29NO2/c1-4-5-6-7-8-9-12-17-14(16)15-11-10-13(2)3/h13H,4-12H2,1-3H3

**InchiKey:** ODMTXLAOWIGNIA-UHFFFAOYSA-N

**Formula:** C14H29NO2

**SMILES:** CCCCCCCCOC(=O)NCCC(C)C

**Mol. weight [g/mol]:** 243.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -79.97 | kJ/mol | Joback Method |
| hf | -528.90 | kJ/mol | Joback Method |
| hfus | 36.38 | kJ/mol | Joback Method |
| hvap | 61.96 | kJ/mol | Joback Method |
| log10ws | -4.47 | | Crippen Method |
| logp | 4.119 | | Crippen Method |
| mcvol | 225.540 | ml/mol | McGowan Method |
| pc | 1606.42 | kPa | Joback Method |
| rinpol | 1784.00 | | NIST Webbook |
| rinpol | 1784.00 | | NIST Webbook |
| tb | 645.74 | K | Joback Method |
| tc | 819.35 | K | Joback Method |
| tf | 357.36 | K | Joback Method |
| vc | 0.873 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 627.76 | J/mol×K | 645.74 | Joback Method |
| cpg | 644.72 | J/mol×K | 674.68 | Joback Method |
| cpg | 660.93 | J/mol×K | 703.61 | Joback Method |
| cpg | 676.38 | J/mol×K | 732.55 | Joback Method |
| cpg | 691.11 | J/mol×K | 761.48 | Joback Method |
| cpg | 705.12 | J/mol×K | 790.42 | Joback Method |
| cpg | 718.42 | J/mol×K | 819.35 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406543&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

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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 |