# Hexanoic acid, 2-dimethylamino, methyl ester

**Inchi:** InChI=1S/C9H19NO2/c1-5-6-7-8(10(2)3)9(11)12-4/h8H,5-7H2,1-4H3
**InchiKey:** OZQUQEWSJJCYPL-UHFFFAOYSA-N
**Formula:** C9H19NO2
**SMILES:** CCCCC(C(=O)OC)N(C)C
**Mol. weight [g/mol]:** 173.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -100.68 | kJ/mol | Joback Method |
| hf | -411.64 | kJ/mol | Joback Method |
| hfus | 21.35 | kJ/mol | Joback Method |
| hvap | 46.44 | kJ/mol | Joback Method |
| log10ws | -1.13 | | Crippen Method |
| logp | 1.280 | | Crippen Method |
| mcvol | 155.090 | ml/mol | McGowan Method |
| pc | 2426.65 | kPa | Joback Method |
| rinpol | 1070.00 | | NIST Webbook |
| rinpol | 1070.00 | | NIST Webbook |
| tb | 493.61 | K | Joback Method |
| tc | 669.14 | K | Joback Method |
| tf | 280.82 | K | Joback Method |
| vc | 0.576 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 356.39 | J/mol×K | 493.61 | Joback Method |
| cpg | 370.77 | J/mol×K | 522.87 | Joback Method |
| cpg | 384.56 | J/mol×K | 552.12 | Joback Method |
| cpg | 397.78 | J/mol×K | 581.38 | Joback Method |
| cpg | 410.42 | J/mol×K | 610.63 | Joback Method |
| cpg | 422.51 | J/mol×K | 639.89 | Joback Method |
| cpg | 434.06 | J/mol×K | 669.14 | 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=R106644&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 |