# DISOPYRAMIDE, M(N-DESALKYL-), AC

**Inchi:** InChI=1S/C18H20N2O2/c1-14(21)20-13-12-18(17(19)22,15-8-4-2-5-9-15)16-10-6-3-7-11
**InchiKey:** SUSVAGLOTXKSAV-UHFFFAOYSA-N
**Formula:** C18H20N2O2
**SMILES:** CC(=O)NCCC(C(N)=O)(c1ccccc1)c1ccccc1
**Mol. weight [g/mol]:** 296.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 226.34 | kJ/mol | Joback Method |
| hf | -88.44 | kJ/mol | Joback Method |
| hfus | 36.54 | kJ/mol | Joback Method |
| hvap | 89.49 | kJ/mol | Joback Method |
| log10ws | -3.51 | | Crippen Method |
| logp | 1.984 | | Crippen Method |
| mcvol | 240.060 | ml/mol | McGowan Method |
| pc | 2336.03 | kPa | Joback Method |
| rinpol | 2640.00 | | NIST Webbook |
| rinpol | 2640.00 | | NIST Webbook |
| tb | 891.81 | K | Joback Method |
| tc | 1138.77 | K | Joback Method |
| tf | 583.66 | K | Joback Method |
| vc | 0.892 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 731.36 | J/mol×K | 891.81 | Joback Method |
| cpg | 744.37 | J/mol×K | 932.97 | Joback Method |
| cpg | 756.29 | J/mol×K | 974.13 | Joback Method |
| cpg | 767.25 | J/mol×K | 1015.29 | Joback Method |
| cpg | 777.40 | J/mol×K | 1056.45 | Joback Method |
| cpg | 786.87 | J/mol×K | 1097.61 | Joback Method |
| cpg | 795.79 | J/mol×K | 1138.77 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R255088&Units=SI |

# 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 |