# Acridan, 2-chloro-9-(3-dimethylaminopropyl)-

**Inchi:** InChI=1S/C18H21ClN2/c1-21(2)11-5-7-14-15-6-3-4-8-17(15)20-18-10-9-13(19)12-16(14)
**InchiKey:** JFRLWWDJCFYFSU-UHFFFAOYSA-N
**Formula:** C18H21ClN2
**SMILES:** CN(C)CCCC1c2ccccc2Nc2ccc(Cl)cc21
**Mol. weight [g/mol]:** 300.83
**CAS:** 5310-55-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 556.02 | kJ/mol | Joback Method |
| hf | 192.36 | kJ/mol | Joback Method |
| hfus | 46.33 | kJ/mol | Joback Method |
| hvap | 75.13 | kJ/mol | Joback Method |
| log10ws | -4.94 | | Crippen Method |
| logp | 4.871 | | Crippen Method |
| mcvol | 238.300 | ml/mol | McGowan Method |
| pc | 1996.55 | kPa | Joback Method |
| tb | 780.43 | K | Joback Method |
| tc | 1013.40 | K | Joback Method |
| tf | 571.90 | K | Joback Method |
| vc | 0.896 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 676.66 | J/mol×K | 780.43 | Joback Method |
| cpg | 693.15 | J/mol×K | 819.26 | Joback Method |
| cpg | 708.54 | J/mol×K | 858.09 | Joback Method |
| cpg | 722.95 | J/mol×K | 896.92 | Joback Method |
| cpg | 736.49 | J/mol×K | 935.75 | Joback Method |
| cpg | 749.26 | J/mol×K | 974.58 | Joback Method |
| cpg | 761.39 | J/mol×K | 1013.40 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C5310554&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

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