# Malonic dilactone, alpha-[2-(diethylamino)ethyl]-cis-1(me),3(h),4(h)-c

**Inchi:** InChI=1S/C19H31NO4/c1-6-20(7-2)11-10-19-14-12-18(5,24-16(19)22)9-8-13(14)17(3,4)2

**InchiKey:** INHWOYUBJKTBSL-UHFFFAOYSA-N

**Formula:** C19H31NO4

**SMILES:** CCN(CC)CCC12C(=O)OC3(C)CCC(C1C3)C(C)(C)OC2=O

**Mol. weight [g/mol]:** 337.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -83.48 | kJ/mol | Joback Method |
| hf | -702.40 | kJ/mol | Joback Method |
| hfus | 34.32 | kJ/mol | Joback Method |
| hvap | 73.63 | kJ/mol | Joback Method |
| log10ws | -3.25 | | Crippen Method |
| logp | 2.772 | | Crippen Method |
| mcvol | 270.850 | ml/mol | McGowan Method |
| pc | 1655.15 | kPa | Joback Method |
| tb | 860.51 | K | Joback Method |
| tc | 1095.08 | K | Joback Method |
| tf | 632.42 | K | Joback Method |
| vc | 1.012 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 955.03 | J/mol×K | 860.51 | Joback Method |
| cpg | 981.82 | J/mol×K | 899.61 | Joback Method |
| cpg | 1009.31 | J/mol×K | 938.70 | Joback Method |
| cpg | 1037.89 | J/mol×K | 977.80 | Joback Method |
| cpg | 1067.93 | J/mol×K | 1016.89 | Joback Method |
| cpg | 1099.81 | J/mol×K | 1055.99 | Joback Method |
| cpg | 1133.91 | J/mol×K | 1095.08 | Joback Method |

# Sources

| | |
|---|---|
| **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=B6006142&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |