# Diethylene glycol, amino, N-octyl

**Inchi:** InChI=1S/C12H27NO2/c1-2-3-4-5-6-7-8-13-9-11-15-12-10-14/h13-14H,2-12H2,1H3
**InchiKey:** YIJHQMHGNQRSNO-UHFFFAOYSA-N
**Formula:** C12H27NO2
**SMILES:** CCCCCCCCNCCOCCO
**Mol. weight [g/mol]:** 217.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -102.27 | kJ/mol | Joback Method |
| hf | -521.99 | kJ/mol | Joback Method |
| hfus | 37.21 | kJ/mol | Joback Method |
| hvap | 67.83 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 1.945 | | Crippen Method |
| mcvol | 201.660 | ml/mol | McGowan Method |
| pc | 1920.30 | kPa | Joback Method |
| rinpol | 1608.00 | | NIST Webbook |
| tb | 638.73 | K | Joback Method |
| tc | 801.24 | K | Joback Method |
| tf | 360.71 | K | Joback Method |
| vc | 0.779 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 563.91 | J/mol×K | 638.73 | Joback Method |
| cpg | 578.43 | J/mol×K | 665.81 | Joback Method |
| cpg | 592.36 | J/mol×K | 692.90 | Joback Method |
| cpg | 605.70 | J/mol×K | 719.98 | Joback Method |
| cpg | 618.48 | J/mol×K | 747.07 | Joback Method |
| cpg | 630.70 | J/mol×K | 774.15 | Joback Method |
| cpg | 642.37 | J/mol×K | 801.24 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R119987&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |