# 3,6-Dimethyl-4-octyn-3,6-diol

| | |
|---|---|
| **Other names:** | 3,6-Dimethyl-4-octyne-3,6-diol |
| | 4-Octyne-3,6-diol, 3,6-dimethyl- |
| | Surfynol 82 |
| | 4-Octyn-3,6-diol, 3,6-dimethyl- |
| | 3,6-Dimethyl-octin-4-diol-(3,6) |
| | Surfynol 82, 82S |
| | 3,6-dimethyloct-4-yne-3,6-diol |
| **Inchi:** | InChI=1S/C10H18O2/c1-5-9(3,11)7-8-10(4,12)6-2/h11-12H,5-6H2,1-4H3 |
| **InchiKey:** | NUYADIDKTLPDGG-UHFFFAOYSA-N |
| **Formula:** | C10H18O2 |
| **SMILES:** | CCC(C)(O)C#CC(C)(O)CC |
| **Mol. weight [g/mol]:** | 170.25 |
| **CAS:** | 78-66-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -31.84 | kJ/mol | Joback Method |
| hf | -299.39 | kJ/mol | Joback Method |
| hfus | 18.13 | kJ/mol | Joback Method |
| hvap | 70.77 | kJ/mol | Joback Method |
| log10ws | -2.55 | | Crippen Method |
| logp | 1.312 | | Crippen Method |
| mcvol | 154.900 | ml/mol | McGowan Method |
| pc | 3100.18 | kPa | Joback Method |
| tb | 615.10 | K | Joback Method |
| tc | 801.74 | K | Joback Method |
| tf | 435.04 | K | Joback Method |
| vc | 0.574 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 407.43 | J/mol×K | 615.10 | Joback Method |
| cpg | 419.01 | J/mol×K | 646.21 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 429.92 | J/mol×K | 677.31 | Joback Method |
| cpg | 440.20 | J/mol×K | 708.42 | Joback Method |
| cpg | 449.89 | J/mol×K | 739.52 | Joback Method |
| cpg | 459.06 | J/mol×K | 770.63 | Joback Method |
| cpg | 467.73 | J/mol×K | 801.74 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 484.20 | K | 90.70 | NIST Webbook |
| tbrp | 375.50 ± 0.50 | K | 0.30 | NIST Webbook |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C78660&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

**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
**tbrp:** Boiling point at reduced pressure
**tc:** Critical Temperature
**tf:** Normal melting (fusion) point

**vc:** Critical Volume