# M-xylene-alpha,alpha'-diol, 2-hydroxy-5-(3-methyl-2-buten-1-yl)-

**Inchi:** InChI=1S/C13H18O3/c1-9(2)3-4-10-5-11(7-14)13(16)12(6-10)8-15/h3,5-6,14-16H,4,7-8H

**InchiKey:** NCWXUUYNQITKOB-UHFFFAOYSA-N

**Formula:** C13H18O3

**SMILES:** CC(C)=CCc1cc(CO)c(O)c(CO)c1

**Mol. weight [g/mol]:** 222.28

**CAS:** 116632-93-0

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -204.86 | kJ/mol | Joback Method |
| hf | -472.40 | kJ/mol | Joback Method |
| hfus | 35.54 | kJ/mol | Joback Method |
| hvap | 94.54 | kJ/mol | Joback Method |
| log10ws | -3.22 | | Crippen Method |
| logp | 1.885 | | Crippen Method |
| mcvol | 183.580 | ml/mol | McGowan Method |
| pc | 3173.97 | kPa | Joback Method |
| tb | 802.50 | K | Joback Method |
| tc | 1002.34 | K | Joback Method |
| tf | 502.05 | K | Joback Method |
| vc | 0.640 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 535.90 | J/mol×K | 802.50 | Joback Method |
| cpg | 546.50 | J/mol×K | 835.81 | Joback Method |
| cpg | 556.70 | J/mol×K | 869.11 | Joback Method |
| cpg | 566.58 | J/mol×K | 902.42 | Joback Method |
| cpg | 576.20 | J/mol×K | 935.73 | Joback Method |
| cpg | 585.64 | J/mol×K | 969.03 | Joback Method |
| cpg | 594.97 | J/mol×K | 1002.34 | 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=C116632930&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 |