# di-(3-Methoxybutyl)glutarate

**Inchi:** InChI=1S/C15H28O6/c1-12(18-3)8-10-20-14(16)6-5-7-15(17)21-11-9-13(2)19-4/h12-13H
**InchiKey:** NMLOQANBHLGBTR-UHFFFAOYSA-N
**Formula:** C15H28O6
**SMILES:** COC(C)CCOC(=O)CCCC(=O)OCCC(C)OC
**Mol. weight [g/mol]:** 304.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -607.30 | kJ/mol | Joback Method |
| hf | -1117.53 | kJ/mol | Joback Method |
| hfus | 35.51 | kJ/mol | Joback Method |
| hvap | 71.34 | kJ/mol | Joback Method |
| log10ws | -2.22 | | Crippen Method |
| logp | 2.093 | | Crippen Method |
| mcvol | 248.830 | ml/mol | McGowan Method |
| pc | 1497.67 | kPa | Joback Method |
| rinpol | 1931.00 | | NIST Webbook |
| tb | 739.14 | K | Joback Method |
| tc | 920.55 | K | Joback Method |
| tf | 417.59 | K | Joback Method |
| vc | 0.948 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 737.27 | J/mol×K | 739.14 | Joback Method |
| cpg | 808.81 | J/mol×K | 890.32 | Joback Method |
| cpg | 796.31 | J/mol×K | 860.08 | Joback Method |
| cpg | 782.89 | J/mol×K | 829.85 | Joback Method |
| cpg | 768.57 | J/mol×K | 799.61 | Joback Method |
| cpg | 753.36 | J/mol×K | 769.38 | Joback Method |
| cpg | 820.39 | J/mol×K | 920.55 | Joback Method |
| dvisc | 0.0000521 | Pa×s | 739.14 | Joback Method |
| dvisc | 0.0000699 | Pa×s | 685.55 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000986 | Pa×s | 631.96 | Joback Method |
| dvisc | 0.0001481 | Pa×s | 578.37 | Joback Method |
| dvisc | 0.0002420 | Pa×s | 524.77 | Joback Method |
| dvisc | 0.0004420 | Pa×s | 471.18 | Joback Method |
| dvisc | 0.0009422 | Pa×s | 417.59 | Joback Method |

# Sources

| | |
|---|---|
| **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=R542228&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |