# Glutaric acid, isobutyl 2-methylpentyl ester

**Inchi:** InChI=1S/C15H28O4/c1-5-7-13(4)11-19-15(17)9-6-8-14(16)18-10-12(2)3/h12-13H,5-11H
**InchiKey:** LAPRDXDUOMXTBN-UHFFFAOYSA-N
**Formula:** C15H28O4
**SMILES:** CCCC(C)COC(=O)CCCC(=O)OCC(C)C
**Mol. weight [g/mol]:** 272.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -397.30 | kJ/mol | Joback Method |
| hf | -853.09 | kJ/mol | Joback Method |
| hfus | 33.13 | kJ/mol | Joback Method |
| hvap | 66.52 | kJ/mol | Joback Method |
| log10ws | -3.34 | | Crippen Method |
| logp | 3.335 | | Crippen Method |
| mcvol | 237.090 | ml/mol | McGowan Method |
| pc | 1537.87 | kPa | Joback Method |
| rinpol | 1812.00 | | NIST Webbook |
| rinpol | 1812.00 | | NIST Webbook |
| tb | 694.30 | K | Joback Method |
| tc | 874.56 | K | Joback Method |
| tf | 373.13 | K | Joback Method |
| vc | 0.911 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 678.23 | J/mol×K | 694.30 | Joback Method |
| cpg | 752.95 | J/mol×K | 844.52 | Joback Method |
| cpg | 739.62 | J/mol×K | 814.47 | Joback Method |
| cpg | 725.49 | J/mol×K | 784.43 | Joback Method |
| cpg | 710.56 | J/mol×K | 754.39 | Joback Method |
| cpg | 694.81 | J/mol×K | 724.34 | Joback Method |
| cpg | 765.47 | J/mol×K | 874.56 | Joback Method |
| dvisc | 0.0000905 | Pa×s | 694.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001227 | Pa×s | 640.77 | Joback Method |
| dvisc | 0.0001760 | Pa×s | 587.24 | Joback Method |
| dvisc | 0.0002714 | Pa×s | 533.71 | Joback Method |
| dvisc | 0.0004608 | Pa×s | 480.19 | Joback Method |
| dvisc | 0.0008937 | Pa×s | 426.66 | Joback Method |
| dvisc | 0.0020958 | Pa×s | 373.13 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358412&Units=SI |

# 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 |