# Glutaric acid, isobutyl 3-(2-methoxyethyl)heptyl ester

**Inchi:** InChI=1S/C19H36O5/c1-5-6-8-17(11-13-22-4)12-14-23-18(20)9-7-10-19(21)24-15-16(2)3

**InchiKey:** ZWTAYHZSXCXSBP-UHFFFAOYSA-N

**Formula:** C19H36O5

**SMILES:** CCCCC(CCOC)CCOC(=O)CCCC(=O)OCC(C)C

**Mol. weight [g/mol]:** 344.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -468.62 | kJ/mol | Joback Method |
| hf | -1067.87 | kJ/mol | Joback Method |
| hfus | 44.68 | kJ/mol | Joback Method |
| hvap | 77.83 | kJ/mol | Joback Method |
| log10ws | -4.10 | | Crippen Method |
| logp | 4.132 | | Crippen Method |
| mcvol | 299.320 | ml/mol | McGowan Method |
| pc | 1148.32 | kPa | Joback Method |
| rinpol | 2281.00 | | NIST Webbook |
| rinpol | 2281.00 | | NIST Webbook |
| tb | 808.24 | K | Joback Method |
| tc | 993.75 | K | Joback Method |
| tf | 440.44 | K | Joback Method |
| vc | 1.153 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 941.23 | J/mol×K | 808.24 | Joback Method |
| cpg | 1019.37 | J/mol×K | 962.83 | Joback Method |
| cpg | 1005.88 | J/mol×K | 931.91 | Joback Method |
| cpg | 991.34 | J/mol×K | 900.99 | Joback Method |
| cpg | 975.71 | J/mol×K | 870.08 | Joback Method |
| cpg | 959.02 | J/mol×K | 839.16 | Joback Method |
| cpg | 1031.79 | J/mol×K | 993.75 | Joback Method |
| dvisc | 0.0000389 | Pa×s | 808.24 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000529 | Pa×s | 746.94 | Joback Method |
| dvisc | 0.0000760 | Pa×s | 685.64 | Joback Method |
| dvisc | 0.0001174 | Pa×s | 624.34 | Joback Method |
| dvisc | 0.0001993 | Pa×s | 563.04 | Joback Method |
| dvisc | 0.0003849 | Pa×s | 501.74 | Joback Method |
| dvisc | 0.0008930 | Pa×s | 440.44 | Joback Method |

# Sources

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|---|---|
| **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=U358521&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 |