

Glutaric acid, isobutyl 4-methylpent-2-yl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C15H28O4/c1-11(2)9-13(5)19-15(17)8-6-7-14(16)18-10-12(3)4/h11-13H,6-10H |
| InchiKey: | WEWCTLQPIRBTPH-UHFFFAOYSA-N |
| Formula: | C15H28O4 |
| SMILES: | CC(C)COC(=O)CCCC(=O)OC(C)CC(C)C |
| Mol. weight [g/mol]: | 272.38 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -399.74 | kJ/mol | Joback Method |
| hf | -858.37 | kJ/mol | Joback Method |
| hfus | 29.61 | kJ/mol | Joback Method |
| hvap | 66.13 | kJ/mol | Joback Method |
| log10ws | -3.45 | | Crippen Method |
| logp | 3.334 | | Crippen Method |
| mvol | 237.090 | ml/mol | McGowan Method |
| pc | 1547.57 | kPa | Joback Method |
| rinpol | 1722.00 | | NIST Webbook |
| rinpol | 1722.00 | | NIST Webbook |
| tb | 693.86 | K | Joback Method |
| tc | 876.51 | K | Joback Method |
| tf | 358.13 | K | Joback Method |
| vc | 0.905 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 678.70 | J/molxK | 693.86 | Joback Method |
| cpg | 754.34 | J/molxK | 846.06 | Joback Method |
| cpg | 740.89 | J/molxK | 815.62 | Joback Method |
| cpg | 726.61 | J/molxK | 785.18 | Joback Method |
| cpg | 711.49 | J/molxK | 754.74 | Joback Method |
| cpg | 695.52 | J/molxK | 724.30 | Joback Method |
| cpg | 766.97 | J/molxK | 876.51 | Joback Method |
| dvisc | 0.0000837 | Paxs | 693.86 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001159 | Paxs | 637.90 | Joback Method |
| dvisc | 0.0001709 | Paxs | 581.95 | Joback Method |
| dvisc | 0.0002735 | Paxs | 526.00 | Joback Method |
| dvisc | 0.0004895 | Paxs | 470.04 | Joback Method |
| dvisc | 0.0010257 | Paxs | 414.08 | Joback Method |
| dvisc | 0.0027078 | Paxs | 358.13 | 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=U359378&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/49-997-2/Glutaric-acid-isobutyl-4-methylpent-2-yl-ester.pdf>

Generated by Cheméo on 2024-04-23 16:16:17.31255922 +0000 UTC m=+16178226.233136532.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.