# Glutaric acid, (2-methylcyclohex-1-enyl)methyl dodec-2-en-1-yl ester

**Inchi:** InChI=1S/C25H42O4/c1-3-4-5-6-7-8-9-10-11-14-20-28-24(26)18-15-19-25(27)29-21-23-1
**InchiKey:** XUOQHJVBXBTUJI-SDNWHVSQSA-N
**Formula:** C25H42O4
**SMILES:** CCCCCCCCCC=CCOC(=O)CCCC(=O)OCC1=C(C)CCCC1
**Mol. weight [g/mol]:** 406.60

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -185.14 | kJ/mol | Joback Method |
| hf | -822.21 | kJ/mol | Joback Method |
| hfus | 57.49 | kJ/mol | Joback Method |
| hvap | 91.87 | kJ/mol | Joback Method |
| log10ws | -7.61 | | Crippen Method |
| logp | 6.831 | | Crippen Method |
| mcvol | 358.530 | ml/mol | McGowan Method |
| pc | 958.51 | kPa | Joback Method |
| rinpol | 2920.00 | | NIST Webbook |
| rinpol | 2920.00 | | NIST Webbook |
| tb | 961.48 | K | Joback Method |
| tc | 1177.15 | K | Joback Method |
| tf | 548.17 | K | Joback Method |
| vc | 1.383 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1215.10 | J/mol×K | 961.48 | Joback Method |
| cpg | 1233.34 | J/mol×K | 997.43 | Joback Method |
| cpg | 1250.14 | J/mol×K | 1033.37 | Joback Method |
| cpg | 1265.56 | J/mol×K | 1069.32 | Joback Method |
| cpg | 1279.65 | J/mol×K | 1105.26 | Joback Method |
| cpg | 1292.46 | J/mol×K | 1141.21 | Joback Method |
| cpg | 1304.06 | J/mol×K | 1177.15 | Joback Method |
| dvisc | 0.0003142 | Pa×s | 548.17 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001525 | Pa×s | 617.05 | Joback Method |
| dvisc | 0.0000855 | Pa×s | 685.94 | Joback Method |
| dvisc | 0.0000533 | Pa×s | 754.83 | Joback Method |
| dvisc | 0.0000360 | Pa×s | 823.71 | Joback Method |
| dvisc | 0.0000258 | Pa×s | 892.60 | Joback Method |
| dvisc | 0.0000194 | Pa×s | 961.48 | 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=U405510&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |