# Glutaric acid, hept-2-yl 2-propylphenyl ester

**Inchi:** InChI=1S/C21H32O4/c1-4-6-7-12-17(3)24-20(22)15-10-16-21(23)25-19-14-9-8-13-18(19)
**InchiKey:** XJARTRUMZBVWNH-UHFFFAOYSA-N
**Formula:** C21H32O4
**SMILES:** CCCCCC(C)OC(=O)CCCC(=O)Oc1ccccc1CCC
**Mol. weight [g/mol]:** 348.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -241.56 | kJ/mol | Joback Method |
| hf | -746.59 | kJ/mol | Joback Method |
| hfus | 45.85 | kJ/mol | Joback Method |
| hvap | 83.20 | kJ/mol | Joback Method |
| log10ws | -6.17 | | Crippen Method |
| logp | 5.227 | | Crippen Method |
| mcvol | 297.870 | ml/mol | McGowan Method |
| pc | 1259.27 | kPa | Joback Method |
| rinpol | 2358.00 | | NIST Webbook |
| rinpol | 2358.00 | | NIST Webbook |
| tb | 863.68 | K | Joback Method |
| tc | 1066.32 | K | Joback Method |
| tf | 494.69 | K | Joback Method |
| vc | 1.145 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 937.65 | J/mol×K | 863.68 | Joback Method |
| cpg | 954.09 | J/mol×K | 897.45 | Joback Method |
| cpg | 969.33 | J/mol×K | 931.23 | Joback Method |
| cpg | 983.39 | J/mol×K | 965.00 | Joback Method |
| cpg | 996.30 | J/mol×K | 998.77 | Joback Method |
| cpg | 1008.08 | J/mol×K | 1032.54 | Joback Method |
| cpg | 1018.76 | J/mol×K | 1066.32 | Joback Method |
| dvisc | 0.0006043 | Pa×s | 494.69 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003060 | Pa×s | 556.19 | Joback Method |
| dvisc | 0.0001775 | Pa×s | 617.69 | Joback Method |
| dvisc | 0.0001136 | Pa×s | 679.18 | Joback Method |
| dvisc | 0.0000783 | Pa×s | 740.68 | Joback Method |
| dvisc | 0.0000571 | Pa×s | 802.18 | Joback Method |
| dvisc | 0.0000436 | Pa×s | 863.68 | Joback Method |

# Sources

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|---|---|
| **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=U392143&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |