# Glutaric acid, 2-(methylthio)phenyl pentyl ester

**Inchi:** InChI=1S/C17H24O4S/c1-3-4-7-13-20-16(18)11-8-12-17(19)21-14-9-5-6-10-15(14)22-2/h

**InchiKey:** HVLSYGZTLSSMCL-UHFFFAOYSA-N

**Formula:** C17H24O4S

**SMILES:** CCCCCOC(=O)CCCC(=O)Oc1ccccc1SC

**Mol. weight [g/mol]:** 324.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -239.68 | kJ/mol | Joback Method |
| hf | -616.88 | kJ/mol | Joback Method |
| hfus | 43.14 | kJ/mol | Joback Method |
| hvap | 81.50 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 4.218 | | Crippen Method |
| mcvol | 257.860 | ml/mol | McGowan Method |
| pc | 1700.50 | kPa | Joback Method |
| rinpol | 2658.00 | | NIST Webbook |
| tb | 841.38 | K | Joback Method |
| tc | 1055.08 | K | Joback Method |
| tf | 499.01 | K | Joback Method |
| vc | 0.982 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 761.89 | J/mol×K | 841.38 | Joback Method |
| cpg | 776.18 | J/mol×K | 877.00 | Joback Method |
| cpg | 789.28 | J/mol×K | 912.61 | Joback Method |
| cpg | 801.20 | J/mol×K | 948.23 | Joback Method |
| cpg | 811.95 | J/mol×K | 983.85 | Joback Method |
| cpg | 821.53 | J/mol×K | 1019.46 | Joback Method |
| cpg | 829.96 | J/mol×K | 1055.08 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377540&Units=SI |
| **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 |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |