

Dimethylmalonic acid, 3-methylphenyl nonyl ester

| | |
|----------------------|--|
| Inchi: | InChI=1S/C21H32O4/c1-5-6-7-8-9-10-11-15-24-19(22)21(3,4)20(23)25-18-14-12-13-17(2) |
| InchiKey: | SZCNTTUAQWNHOB-UHFFFAOYSA-N |
| Formula: | C21H32O4 |
| SMILES: | CCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C)c1 |
| Mol. weight [g/mol]: | 348.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -236.28 | kJ/mol | Joback Method |
| hf | -750.06 | kJ/mol | Joback Method |
| hfus | 41.96 | kJ/mol | Joback Method |
| hvap | 82.29 | kJ/mol | Joback Method |
| log10ws | -5.90 | | Crippen Method |
| logp | 5.220 | | Crippen Method |
| mcvol | 297.870 | ml/mol | McGowan Method |
| pc | 1269.16 | kPa | Joback Method |
| rinsol | 2291.00 | | NIST Webbook |
| tb | 860.89 | K | Joback Method |
| tc | 1066.30 | K | Joback Method |
| tf | 512.11 | K | Joback Method |
| vc | 1.141 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 937.93 | J/molxK | 860.89 | Joback Method |
| cpg | 1008.90 | J/molxK | 1032.07 | Joback Method |
| cpg | 996.89 | J/molxK | 997.83 | Joback Method |
| cpg | 983.83 | J/molxK | 963.60 | Joback Method |
| cpg | 969.67 | J/molxK | 929.36 | Joback Method |
| cpg | 954.39 | J/molxK | 895.13 | Joback Method |
| cpg | 1019.92 | J/molxK | 1066.30 | Joback Method |
| dvisc | 0.0000374 | Paxs | 860.89 | Joback Method |
| dvisc | 0.0000492 | Paxs | 802.76 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000674 | Paxs | 744.63 | Joback Method |
| dvisc | 0.0000975 | Paxs | 686.50 | Joback Method |
| dvisc | 0.0001510 | Paxs | 628.37 | Joback Method |
| dvisc | 0.0002558 | Paxs | 570.24 | Joback Method |
| dvisc | 0.0004882 | Paxs | 512.11 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U363617&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 |

Latest version available from:

<https://www.chemeo.com/cid/57-471-6/Dimethylmalonic-acid-3-methylphenyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-25 22:05:02.386128786 +0000 UTC m=+16371951.306706159.

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