

Diglycolic acid, 2,5-dimethylphenyl nonyl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C21H32O5/c1-4-5-6-7-8-9-10-13-25-20(22)15-24-16-21(23)26-19-14-17(2)11- |
| InchiKey: | VVWURGOBJXHKLKLP-UHFFFAOYSA-N |
| Formula: | C21H32O5 |
| SMILES: | CCCCCCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C |
| Mol. weight [g/mol]: | 364.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -353.75 | kJ/mol | Joback Method |
| hf | -885.00 | kJ/mol | Joback Method |
| hfus | 50.17 | kJ/mol | Joback Method |
| hvap | 86.66 | kJ/mol | Joback Method |
| log10ws | -5.29 | | Crippen Method |
| logp | 4.519 | | Crippen Method |
| mvol | 303.740 | ml/mol | McGowan Method |
| pc | 1224.27 | kPa | Joback Method |
| rinpol | 3204.00 | | NIST Webbook |
| rinpol | 3204.00 | | NIST Webbook |
| tb | 891.52 | K | Joback Method |
| tc | 1095.88 | K | Joback Method |
| tf | 544.44 | K | Joback Method |
| vc | 1.169 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 966.06 | J/molxK | 891.52 | Joback Method |
| cpg | 1031.86 | J/molxK | 1061.82 | Joback Method |
| cpg | 1021.25 | J/molxK | 1027.76 | Joback Method |
| cpg | 1009.38 | J/molxK | 993.70 | Joback Method |
| cpg | 996.22 | J/molxK | 959.64 | Joback Method |
| cpg | 981.79 | J/molxK | 925.58 | Joback Method |
| cpg | 1041.21 | J/molxK | 1095.88 | Joback Method |
| dvisc | 0.0000362 | Paxs | 891.52 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000460 | Paxs | 833.67 | Joback Method |
| dvisc | 0.0000606 | Paxs | 775.83 | Joback Method |
| dvisc | 0.0000834 | Paxs | 717.98 | Joback Method |
| dvisc | 0.0001214 | Paxs | 660.13 | Joback Method |
| dvisc | 0.0001899 | Paxs | 602.29 | Joback Method |
| dvisc | 0.0003268 | Paxs | 544.44 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U382711&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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/87-190-5/Diglycolic-acid-2-5-dimethylphenyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-25 06:44:34.317922318 +0000 UTC m=+16316723.238499634.

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