

Succinic acid, ethyl 2-tertbutyl-6-methylphenyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C17H24O4/c1-6-20-14(18)10-11-15(19)21-16-12(2)8-7-9-13(16)17(3,4)5/h7-9H |
| InchiKey: | VWVUCNYMGRFTJX-UHFFFAOYSA-N |
| Formula: | C17H24O4 |
| SMILES: | CCOC(=O)CCC(=O)Oc1c(C)cccc1C(C)(C)C |
| Mol. weight [g/mol]: | 292.37 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -279.59 | kJ/mol | Joback Method |
| hf | -678.97 | kJ/mol | Joback Method |
| hfus | 31.21 | kJ/mol | Joback Method |
| hvap | 74.05 | kJ/mol | Joback Method |
| log10ws | -4.11 | | Crippen Method |
| logp | 3.541 | | Crippen Method |
| mvol | 241.510 | ml/mol | McGowan Method |
| pc | 1682.41 | kPa | Joback Method |
| rinpol | 1991.00 | | NIST Webbook |
| rinpol | 1991.00 | | NIST Webbook |
| tb | 774.35 | K | Joback Method |
| tc | 983.43 | K | Joback Method |
| tf | 479.55 | K | Joback Method |
| vc | 0.916 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 705.40 | J/molxK | 774.35 | Joback Method |
| cpg | 773.05 | J/molxK | 948.59 | Joback Method |
| cpg | 761.55 | J/molxK | 913.74 | Joback Method |
| cpg | 749.06 | J/molxK | 878.89 | Joback Method |
| cpg | 735.56 | J/molxK | 844.04 | Joback Method |
| cpg | 721.02 | J/molxK | 809.20 | Joback Method |
| cpg | 783.59 | J/molxK | 983.43 | Joback Method |
| dvisc | 0.0000670 | Paxs | 774.35 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000858 | Paxs | 725.22 | Joback Method |
| dvisc | 0.0001138 | Paxs | 676.08 | Joback Method |
| dvisc | 0.0001578 | Paxs | 626.95 | Joback Method |
| dvisc | 0.0002313 | Paxs | 577.82 | Joback Method |
| dvisc | 0.0003639 | Paxs | 528.68 | Joback Method |
| dvisc | 0.0006285 | Paxs | 479.55 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349635&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

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| m_{cvol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rin_{pol}: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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