

Sebacic acid, di(2,5-dimethylphenyl) ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C26H34O4/c1-19-13-15-21(3)23(17-19)29-25(27)11-9-7-5-6-8-10-12-26(28)30 |
| InchiKey: | SEEYNLZPKCUITK-UHFFFAOYSA-N |
| Formula: | C26H34O4 |
| SMILES: | <chem>Cc1ccc(C)c(OC(=O)CCCCCCCCC(=O)Oc2cc(C)ccc2C)c1</chem> |
| Mol. weight [g/mol]: | 410.55 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -113.50 | kJ/mol | Joback Method |
| hf | -642.39 | kJ/mol | Joback Method |
| hfus | 55.20 | kJ/mol | Joback Method |
| hvap | 98.98 | kJ/mol | Joback Method |
| log10ws | -8.16 | | Crippen Method |
| logp | 6.552 | | Crippen Method |
| mvol | 344.560 | ml/mol | McGowan Method |
| pc | 1096.44 | kPa | Joback Method |
| rinpol | 3215.00 | | NIST Webbook |
| rinpol | 3215.00 | | NIST Webbook |
| tb | 1020.14 | K | Joback Method |
| tc | 1250.34 | K | Joback Method |
| tf | 630.02 | K | Joback Method |
| vc | 1.323 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1134.56 | J/molxK | 1020.14 | Joback Method |
| cpg | 1189.56 | J/molxK | 1211.98 | Joback Method |
| cpg | 1181.56 | J/molxK | 1173.61 | Joback Method |
| cpg | 1172.11 | J/molxK | 1135.24 | Joback Method |
| cpg | 1161.15 | J/molxK | 1096.87 | Joback Method |
| cpg | 1148.65 | J/molxK | 1058.51 | Joback Method |
| cpg | 1196.14 | J/molxK | 1250.34 | Joback Method |
| dvisc | 0.0000256 | Paxs | 1020.14 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000320 | Paxs | 955.12 | Joback Method |
| dvisc | 0.0000414 | Paxs | 890.10 | Joback Method |
| dvisc | 0.0000557 | Paxs | 825.08 | Joback Method |
| dvisc | 0.0000789 | Paxs | 760.06 | Joback Method |
| dvisc | 0.0001192 | Paxs | 695.04 | Joback Method |
| dvisc | 0.0001962 | Paxs | 630.02 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354984&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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