

Sebacic acid, heptyl 4-nitrophenyl ester

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| Inchi: | InChI=1S/C23H35NO6/c1-2-3-4-9-12-19-29-22(25)13-10-7-5-6-8-11-14-23(26)30-21-17- |
| InchiKey: | ALBARZRUFVIXAI-UHFFFAOYSA-N |
| Formula: | C23H35NO6 |
| SMILES: | CCCCCCCC(=O)CCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1 |
| Mol. weight [g/mol]: | 421.53 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -186.73 | kJ/mol | Joback Method |
| hf | -793.35 | kJ/mol | Joback Method |
| hfus | 65.91 | kJ/mol | Joback Method |
| hvap | 104.63 | kJ/mol | Joback Method |
| log10ws | -7.58 | | Crippen Method |
| logp | 6.135 | | Crippen Method |
| mvol | 343.470 | ml/mol | McGowan Method |
| pc | 1106.68 | kPa | Joback Method |
| rinpol | 3355.00 | | NIST Webbook |
| rinpol | 3355.00 | | NIST Webbook |
| tb | 1061.72 | K | Joback Method |
| tc | 1300.03 | K | Joback Method |
| tf | 675.84 | K | Joback Method |
| vc | 1.345 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|---------|---------|-----------------|---------------|
| cpg | 1169.01 | J/molxK | 1061.72 | Joback Method |
| cpg | 1181.96 | J/molxK | 1101.44 | Joback Method |
| cpg | 1193.35 | J/molxK | 1141.16 | Joback Method |
| cpg | 1203.22 | J/molxK | 1180.88 | Joback Method |
| cpg | 1211.64 | J/molxK | 1220.59 | Joback Method |
| cpg | 1218.67 | J/molxK | 1260.31 | Joback Method |
| cpg | 1224.35 | J/molxK | 1300.03 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354790&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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 |
| h vap: | 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 |
| r in 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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