# Sebacic acid, 4-isopropylphenyl octyl ester

**Inchi:** InChI=1S/C27H44O4/c1-4-5-6-7-12-15-22-30-26(28)16-13-10-8-9-11-14-17-27(29)31-25
**InchiKey:** YOOYFMWMEVIZRZ-UHFFFAOYSA-N
**Formula:** C27H44O4
**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)C)cc1
**Mol. weight [g/mol]:** 432.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -191.04 | kJ/mol | Joback Method |
| hf | -870.43 | kJ/mol | Joback Method |
| hfus | 61.39 | kJ/mol | Joback Method |
| hvap | 96.56 | kJ/mol | Joback Method |
| log10ws | -8.53 | | Crippen Method |
| logp | 7.740 | | Crippen Method |
| mcvol | 382.410 | ml/mol | McGowan Method |
| pc | 868.11 | kPa | Joback Method |
| rinpol | 3249.00 | | NIST Webbook |
| rinpol | 3249.00 | | NIST Webbook |
| tb | 1000.96 | K | Joback Method |
| tc | 1226.87 | K | Joback Method |
| tf | 562.31 | K | Joback Method |
| vc | 1.482 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1306.77 | J/mol×K | 1000.96 | Joback Method |
| cpg | 1324.54 | J/mol×K | 1038.61 | Joback Method |
| cpg | 1340.65 | J/mol×K | 1076.26 | Joback Method |
| cpg | 1355.17 | J/mol×K | 1113.92 | Joback Method |
| cpg | 1368.14 | J/mol×K | 1151.57 | Joback Method |
| cpg | 1379.63 | J/mol×K | 1189.22 | Joback Method |
| cpg | 1389.70 | J/mol×K | 1226.87 | Joback Method |
| dvisc | 0.0002962 | Pa×s | 562.31 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001415 | Pa×s | 635.42 | Joback Method |
| dvisc | 0.0000788 | Pa×s | 708.53 | Joback Method |
| dvisc | 0.0000489 | Pa×s | 781.63 | Joback Method |
| dvisc | 0.0000330 | Pa×s | 854.74 | Joback Method |
| dvisc | 0.0000236 | Pa×s | 927.85 | Joback Method |
| dvisc | 0.0000178 | Pa×s | 1000.96 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354458&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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 |

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