# Isophthalic acid, hexyl 2-isopropylphenyl ester

**Inchi:** InChI=1S/C23H28O4/c1-4-5-6-9-15-26-22(24)18-11-10-12-19(16-18)23(25)27-21-14-8-7
**InchiKey:** AETCFYJPDMOTPD-UHFFFAOYSA-N
**Formula:** C23H28O4
**SMILES:** CCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C(C)C)c1
**Mol. weight [g/mol]:** 368.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -121.94 | kJ/mol | Joback Method |
| hf | -562.81 | kJ/mol | Joback Method |
| hfus | 44.68 | kJ/mol | Joback Method |
| hvap | 90.59 | kJ/mol | Joback Method |
| log10ws | -7.08 | | Crippen Method |
| logp | 5.766 | | Crippen Method |
| mcvol | 302.290 | ml/mol | McGowan Method |
| pc | 1377.86 | kPa | Joback Method |
| rinpol | 2810.00 | | NIST Webbook |
| rinpol | 2810.00 | | NIST Webbook |
| tb | 941.10 | K | Joback Method |
| tc | 1165.57 | K | Joback Method |
| tf | 556.17 | K | Joback Method |
| vc | 1.149 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 956.42 | J/mol×K | 941.10 | Joback Method |
| cpg | 970.76 | J/mol×K | 978.51 | Joback Method |
| cpg | 983.70 | J/mol×K | 1015.92 | Joback Method |
| cpg | 995.28 | J/mol×K | 1053.33 | Joback Method |
| cpg | 1005.54 | J/mol×K | 1090.75 | Joback Method |
| cpg | 1014.52 | J/mol×K | 1128.16 | Joback Method |
| cpg | 1022.27 | J/mol×K | 1165.57 | Joback Method |
| dvisc | 0.0003644 | Pa×s | 556.17 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002004 | Pa×s | 620.33 | Joback Method |
| dvisc | 0.0001233 | Pa×s | 684.48 | Joback Method |
| dvisc | 0.0000824 | Pa×s | 748.63 | Joback Method |
| dvisc | 0.0000587 | Pa×s | 812.79 | Joback Method |
| dvisc | 0.0000440 | Pa×s | 876.94 | Joback Method |
| dvisc | 0.0000343 | Pa×s | 941.10 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344636&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |