

Sebacic acid, isohexyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C25H40O4/c1-20(2)12-11-19-28-24(26)13-9-7-5-6-8-10-14-25(27)29-23-17-15
InchiKey:	DPWUHFFCECPCNV-UHFFFAOYSA-N
Formula:	C25H40O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCC(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	404.58

Physical Properties

Property code	Value	Unit	Source
gf	-210.32	kJ/mol	Joback Method
hf	-834.43	kJ/mol	Joback Method
hfus	52.69	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	6.816		Crippen Method
mvol	354.230	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	3002.00		NIST Webbook
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tb	954.76	K	Joback Method
tc	1169.19	K	Joback Method
tf	524.77	K	Joback Method
vc	1.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.11	J/molxK	954.76	Joback Method
cpg	1199.33	J/molxK	990.50	Joback Method
cpg	1215.06	J/molxK	1026.24	Joback Method
cpg	1229.37	J/molxK	1061.98	Joback Method
cpg	1242.28	J/molxK	1097.71	Joback Method
cpg	1253.86	J/molxK	1133.45	Joback Method
cpg	1264.13	J/molxK	1169.19	Joback Method
dvisc	0.0004286	Paxs	524.77	Joback Method

dvisc	0.0001941	Paxs	596.43	Joback Method
dvisc	0.0001042	Paxs	668.10	Joback Method
dvisc	0.0000631	Paxs	739.76	Joback Method
dvisc	0.0000418	Paxs	811.43	Joback Method
dvisc	0.0000295	Paxs	883.09	Joback Method
dvisc	0.0000220	Paxs	954.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354455&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
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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