

Isophthalic acid, isohexyl 2-propylphenyl ester

Inchi:	InChI=1S/C23H28O4/c1-4-9-18-11-5-6-14-21(18)27-23(25)20-13-7-12-19(16-20)22(24)2
InchiKey:	NLFDMCCBRRFAPQ-UHFFFAOYSA-N
Formula:	C23H28O4
SMILES:	CCCCc1cccc1OC(=O)c1cccc(C(=O)OCCCC(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	-6.87		Crippen Method
logp	5.451		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	2719.00		NIST Webbook
rinpol	2719.00		NIST Webbook
tb	941.10	K	Joback Method
tc	1165.57	K	Joback Method
tf	556.17	K	Joback Method
vc	1.149	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.42	J/molxK	941.10	Joback Method
cpg	970.76	J/molxK	978.51	Joback Method
cpg	983.70	J/molxK	1015.92	Joback Method
cpg	995.28	J/molxK	1053.33	Joback Method
cpg	1005.54	J/molxK	1090.75	Joback Method
cpg	1014.52	J/molxK	1128.16	Joback Method
cpg	1022.27	J/molxK	1165.57	Joback Method
dvisc	0.0003644	Paxs	556.17	Joback Method

dvisc	0.0002004	Paxs	620.33	Joback Method
dvisc	0.0001233	Paxs	684.48	Joback Method
dvisc	0.0000824	Paxs	748.63	Joback Method
dvisc	0.0000587	Paxs	812.79	Joback Method
dvisc	0.0000440	Paxs	876.94	Joback Method
dvisc	0.0000343	Paxs	941.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356628&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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