

Isophthalic acid, isohexyl oct-3-en-2-yl ester

Inchi:	InChI=1S/C22H32O4/c1-5-6-7-8-12-18(4)26-22(24)20-14-9-13-19(16-20)21(23)25-15-10
InchiKey:	KATFQFHIPFJSFA-XYOKQWHBSA-N
Formula:	C22H32O4
SMILES:	CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]:	360.49

Physical Properties

Property code	Value	Unit	Source
gf	-155.36	kJ/mol	Joback Method
hf	-655.29	kJ/mol	Joback Method
hfus	45.12	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.571		Crippen Method
mvol	307.660	ml/mol	McGowan Method
pc	1227.70	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	890.28	K	Joback Method
tc	1099.25	K	Joback Method
tf	485.88	K	Joback Method
vc	1.175	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.00	J/molxK	890.28	Joback Method
cpg	1040.84	J/molxK	1064.42	Joback Method
cpg	1029.11	J/molxK	1029.59	Joback Method
cpg	1016.30	J/molxK	994.76	Joback Method
cpg	1002.38	J/molxK	959.94	Joback Method
cpg	987.29	J/molxK	925.11	Joback Method
cpg	1051.54	J/molxK	1099.25	Joback Method
dvisc	0.0000301	Paxs	890.28	Joback Method

dvisc	0.0000403	Paxs	822.88	Joback Method
dvisc	0.0000567	Paxs	755.48	Joback Method
dvisc	0.0000853	Paxs	688.08	Joback Method
dvisc	0.0001404	Paxs	620.68	Joback Method
dvisc	0.0002606	Paxs	553.28	Joback Method
dvisc	0.0005744	Paxs	485.88	Joback Method

Sources

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=U343894&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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