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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.00	J/mol×K	890.28	Joback Method
cpg	987.29	J/mol×K	925.11	Joback Method
cpg	1002.38	J/mol×K	959.94	Joback Method
cpg	1016.30	J/mol×K	994.76	Joback Method
cpg	1029.11	J/mol×K	1029.59	Joback Method
cpg	1040.84	J/mol×K	1064.42	Joback Method
cpg	1051.54	J/mol×K	1099.25	Joback Method
dvisc	0.0005744	Pa×s	485.88	Joback Method

dvisc	0.0002606	Pa×s	553.28	Joback Method
dvisc	0.0001404	Pa×s	620.68	Joback Method
dvisc	0.0000853	Pa×s	688.08	Joback Method
dvisc	0.0000567	Pa×s	755.48	Joback Method
dvisc	0.0000403	Pa×s	822.88	Joback Method
dvisc	0.0000301	Pa×s	890.28	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343894&Units=SI

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