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

Inchi: InChI=1S/C22H32O4/c1-4-6-8-10-13-18(3)26-22(24)20-15-12-14-19(17-20)21(23)25-16-
InchiKey: RXNBCKGRYOROAL-JLHYYAGUSA-N
Formula: C22H32O4
SMILES: CCCCC=CC(C)OC(=O)c1cccc(C(=O)OCCCCCC)c1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-152.92	kJ/mol	Joback Method
hf	-650.01	kJ/mol	Joback Method
hfus	48.64	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.715		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	890.72	K	Joback Method
tc	1098.22	K	Joback Method
tf	500.88	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.52	J/mol×K	890.72	Joback Method
cpg	986.72	J/mol×K	925.30	Joback Method
cpg	1001.75	J/mol×K	959.89	Joback Method
cpg	1015.64	J/mol×K	994.47	Joback Method
cpg	1028.44	J/mol×K	1029.05	Joback Method
cpg	1040.19	J/mol×K	1063.63	Joback Method
cpg	1050.94	J/mol×K	1098.22	Joback Method
dvisc	0.0005015	Pa×s	500.88	Joback Method

dvisc	0.0002455	Pa×s	565.85	Joback Method
dvisc	0.0001393	Pa×s	630.83	Joback Method
dvisc	0.0000878	Pa×s	695.80	Joback Method
dvisc	0.0000599	Pa×s	760.77	Joback Method
dvisc	0.0000434	Pa×s	825.75	Joback Method
dvisc	0.0000330	Pa×s	890.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343895&Units=SI
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

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