Isophthalic acid, di(oct-3-en-2-yl) ester

Inchi: InChI=1S/C24H34O4/c1-5-7-9-11-14-19(3)27-23(25)21-16-13-17-22(18-21)24(26)28-20(
InchiKey: UJQJWYDVNCDQCN-LCPPQYOVSA-N
Formula: C24H34O4
SMILES: CCCCC=CC(C)OC(=O)c1cccc(C(=O)OC(C)C=CCCCC)c1
Mol. weight [g/mol]: 386.52

Physical Properties

Property code	Value	Unit	Source
gf	-58.30	kJ/mol	Joback Method
hf	-579.35	kJ/mol	Joback Method
hfus	50.50	kJ/mol	Joback Method
hvap	89.41	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.270		Crippen Method
mcvol	331.540	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2697.00		NIST Webbook
rinpol	2697.00		NIST Webbook
tb	940.20	K	Joback Method
tc	1155.71	K	Joback Method
tf	503.34	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.34	J/mol×K	940.20	Joback Method
cpg	1080.68	J/mol×K	976.12	Joback Method
cpg	1095.85	J/mol×K	1012.04	Joback Method
cpg	1109.92	J/mol×K	1047.96	Joback Method
cpg	1122.95	J/mol×K	1083.88	Joback Method
cpg	1135.01	J/mol×K	1119.80	Joback Method
cpg	1146.16	J/mol×K	1155.71	Joback Method
dvisc	0.0004203	Pa×s	503.34	Joback Method

dvisc	0.0001827	Pa×s	576.15	Joback Method
dvisc	0.0000958	Pa×s	648.96	Joback Method
dvisc	0.0000572	Pa×s	721.77	Joback Method
dvisc	0.0000375	Pa×s	794.58	Joback Method
dvisc	0.0000264	Pa×s	867.39	Joback Method
dvisc	0.0000197	Pa×s	940.20	Joback Method

Sources

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=U343896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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