Isophthalic acid, 10-chlorodecyl isohexyl ester

Inchi: InChI=1S/C24H37ClO4/c1-20(2)13-12-18-29-24(27)22-15-11-14-21(19-22)23(26)28-17-1
InchiKey: AZVFSAKVZVWIDY-UHFFFAOYSA-N
Formula: C24H37ClO4
SMILES: CC(C)CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCl)c1
Mol. weight [g/mol]: 425.00

Physical Properties

Property code	Value	Unit	Source
gf	-228.23	kJ/mol	Joback Method
hf	-824.25	kJ/mol	Joback Method
hfus	57.82	kJ/mol	Joback Method
hvap	94.26	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	6.796		Crippen Method
mcvol	352.380	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
tb	969.75	K	Joback Method
tc	1187.41	K	Joback Method
tf	558.42	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.50	J/mol×K	969.75	Joback Method
cpg	1211.85	J/mol×K	1151.14	Joback Method
cpg	1201.44	J/mol×K	1114.86	Joback Method
cpg	1189.75	J/mol×K	1078.58	Joback Method
cpg	1176.72	J/mol×K	1042.30	Joback Method
cpg	1162.32	J/mol×K	1006.03	Joback Method
cpg	1221.01	J/mol×K	1187.41	Joback Method
dvisc	0.0000237	Pa×s	969.75	Joback Method

dvisc	0.0000312	Pa×s	901.19	Joback Method
dvisc	0.0000429	Pa×s	832.64	Joback Method
dvisc	0.0000625	Pa×s	764.09	Joback Method
dvisc	0.0000982	Pa×s	695.53	Joback Method
dvisc	0.0001702	Pa×s	626.98	Joback Method
dvisc	0.0003376	Pa×s	558.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356417&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