Phthalic acid, 2-chloropropyl octadecyl ester

Inchi: InChI=1S/C29H47ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-33-28(31)26-21
InchiKey: OHSXFUARBDKWCO-UHFFFAOYSA-N
Formula: C29H47ClO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)Cl
Mol. weight [g/mol]: 495.13

Physical Properties

Property code	Value	Unit	Source
gf	-186.13	kJ/mol	Joback Method
hf	-927.45	kJ/mol	Joback Method
hfus	70.77	kJ/mol	Joback Method
hvap	105.39	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	8.889		Crippen Method
mcvol	422.830	ml/mol	McGowan Method
pc	761.84	kPa	Joback Method
rinpol	3477.00		NIST Webbook
rinpol	3477.00		NIST Webbook
tb	1084.15	K	Joback Method
tc	1338.81	K	Joback Method
tf	614.77	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1458.17	J/mol×K	1084.15	Joback Method
cpg	1475.39	J/mol×K	1126.59	Joback Method
cpg	1490.60	J/mol×K	1169.04	Joback Method
cpg	1503.92	J/mol×K	1211.48	Joback Method
cpg	1515.44	J/mol×K	1253.93	Joback Method
cpg	1525.25	J/mol×K	1296.37	Joback Method
cpg	1533.47	J/mol×K	1338.81	Joback Method
dvisc	0.0001761	Pa×s	614.77	Joback Method

dvisc	0.0000850	Pa×s	693.00	Joback Method
dvisc	0.0000475	Pa×s	771.23	Joback Method
dvisc	0.0000296	Pa×s	849.46	Joback Method
dvisc	0.0000200	Pa×s	927.69	Joback Method
dvisc	0.0000143	Pa×s	1005.92	Joback Method
dvisc	0.0000108	Pa×s	1084.15	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=U356839&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