Phthalic acid, 2-chloropropyl dodecyl ester

Inchi: InChI=1S/C23H35ClO4/c1-3-4-5-6-7-8-9-10-11-14-17-27-22(25)20-15-12-13-16-21(20)23
InchiKey: RCRSXBSGHRCJAP-UHFFFAOYSA-N
Formula: C23H35ClO4
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)Cl
Mol. weight [g/mol]: 410.98

Physical Properties

Property code	Value	Unit	Source
gf	-236.65	kJ/mol	Joback Method
hf	-803.61	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	92.04	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	6.548		Crippen Method
mcvol	338.290	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	2863.00		NIST Webbook
rinpol	2863.00		NIST Webbook
tb	946.87	K	Joback Method
tc	1160.48	K	Joback Method
tf	547.15	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.40	J/mol×K	946.87	Joback Method
cpg	1150.38	J/mol×K	1124.88	Joback Method
cpg	1139.93	J/mol×K	1089.28	Joback Method
cpg	1128.24	J/mol×K	1053.67	Joback Method
cpg	1115.28	J/mol×K	1018.07	Joback Method
cpg	1101.01	J/mol×K	982.47	Joback Method
cpg	1159.65	J/mol×K	1160.48	Joback Method
dvisc	0.0000276	Pa×s	946.87	Joback Method

dvisc	0.0000362	Pa×s	880.25	Joback Method
dvisc	0.0000497	Pa×s	813.63	Joback Method
dvisc	0.0000722	Pa×s	747.01	Joback Method
dvisc	0.0001128	Pa×s	680.39	Joback Method
dvisc	0.0001942	Pa×s	613.77	Joback Method
dvisc	0.0003816	Pa×s	547.15	Joback Method

Sources

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=U356833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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