Phthalic acid, di(2-chloropropyl) ester

Inchi: InChI=1S/C14H16Cl2O4/c1-9(15)7-19-13(17)11-5-3-4-6-12(11)14(18)20-8-10(2)16/h3-6,
InchiKey: BUADCYGKCVEWBG-UHFFFAOYSA-N
Formula: C14H16Cl2O4
SMILES: CC(Cl)COC(=O)c1ccccc1C(=O)OCC(C)Cl
Mol. weight [g/mol]: 319.18

Physical Properties

Property code	Value	Unit	Source
gf	-326.80	kJ/mol	Joback Method
hf	-638.87	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	76.00	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.255		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	777.94	K	Joback Method
tc	997.29	K	Joback Method
tf	460.64	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.47	J/mol×K	777.94	Joback Method
cpg	604.08	J/mol×K	814.50	Joback Method
cpg	615.67	J/mol×K	851.06	Joback Method
cpg	626.26	J/mol×K	887.61	Joback Method
cpg	635.86	J/mol×K	924.17	Joback Method
cpg	644.49	J/mol×K	960.73	Joback Method
cpg	652.16	J/mol×K	997.29	Joback Method
dvisc	0.0009319	Pa×s	460.64	Joback Method

dvisc	0.0005022	Pa×s	513.52	Joback Method
dvisc	0.0003037	Pa×s	566.41	Joback Method
dvisc	0.0002002	Pa×s	619.29	Joback Method
dvisc	0.0001409	Pa×s	672.17	Joback Method
dvisc	0.0001043	Pa×s	725.06	Joback Method
dvisc	0.0000805	Pa×s	777.94	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=U356840&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