Terephthalic acid, 2-chloropropyl propyl ester

Inchi: InChI=1S/C14H17ClO4/c1-3-8-18-13(16)11-4-6-12(7-5-11)14(17)19-9-10(2)15/h4-7,10H,
InchiKey: NIPYFIAVKUHJBC-UHFFFAOYSA-N
Formula: C14H17ClO4
SMILES: CCCOC(=O)c1ccc(C(=O)OCC(C)Cl)cc1
Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-312.43	kJ/mol	Joback Method
hf	-617.85	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	72.01	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.038		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	740.95	K	Joback Method
tc	953.69	K	Joback Method
tf	445.72	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.56	J/mol×K	740.95	Joback Method
cpg	580.10	J/mol×K	776.41	Joback Method
cpg	592.69	J/mol×K	811.86	Joback Method
cpg	604.33	J/mol×K	847.32	Joback Method
cpg	615.04	J/mol×K	882.78	Joback Method
cpg	624.82	J/mol×K	918.24	Joback Method
cpg	633.68	J/mol×K	953.69	Joback Method
dvisc	0.0009754	Pa×s	445.72	Joback Method

dvisc	0.0005515	Pa×s	494.93	Joback Method
dvisc	0.0003457	Pa×s	544.13	Joback Method
dvisc	0.0002341	Pa×s	593.34	Joback Method
dvisc	0.0001683	Pa×s	642.54	Joback Method
dvisc	0.0001268	Pa×s	691.75	Joback Method
dvisc	0.0000992	Pa×s	740.95	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=U356168&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