

Phthalic acid, 2-chloropropyl propyl ester

Inchi:	InChI=1S/C14H17ClO4/c1-3-8-18-13(16)11-6-4-5-7-12(11)14(17)19-9-10(2)15/h4-7,10H,
InchiKey:	ODPUOYIERVGLFO-UHFFFAOYSA-N
Formula:	C14H17ClO4
SMILES:	CCCOC(=O)c1ccccc1C(=O)OCC(C)Cl
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
mvol	211.480	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1958.00		NIST Webbook
rinpol	1958.00		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/molxK	740.95	Joback Method
cpg	580.10	J/molxK	776.41	Joback Method
cpg	592.69	J/molxK	811.86	Joback Method
cpg	604.33	J/molxK	847.32	Joback Method
cpg	615.04	J/molxK	882.78	Joback Method
cpg	624.82	J/molxK	918.24	Joback Method
cpg	633.68	J/molxK	953.69	Joback Method
dvisc	0.0009754	Paxs	445.72	Joback Method

dvisc	0.0005515	Paxs	494.93	Joback Method
dvisc	0.0003457	Paxs	544.13	Joback Method
dvisc	0.0002341	Paxs	593.34	Joback Method
dvisc	0.0001683	Paxs	642.54	Joback Method
dvisc	0.0001268	Paxs	691.75	Joback Method
dvisc	0.0000992	Paxs	740.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356823&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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