Phthalic acid, 2,2-dichloroethyl propyl ester

Inchi: InChI=1S/C13H14Cl2O4/c1-2-7-18-12(16)9-5-3-4-6-10(9)13(17)19-8-11(14)15/h3-6,11H,
InchiKey: PJHMRLLNEJMCHO-UHFFFAOYSA-N
Formula: C13H14Cl2O4
SMILES: CCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 305.15

Physical Properties

Property code	Value	Unit	Source
gf	-332.78	kJ/mol	Joback Method
hf	-612.95	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	74.16	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.214		Crippen Method
mcvol	209.630	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	755.50	K	Joback Method
tc	974.24	K	Joback Method
tf	464.37	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.54	J/mol×K	755.50	Joback Method
cpg	549.56	J/mol×K	791.96	Joback Method
cpg	560.64	J/mol×K	828.41	Joback Method
cpg	570.80	J/mol×K	864.87	Joback Method
cpg	580.05	J/mol×K	901.33	Joback Method
cpg	588.39	J/mol×K	937.78	Joback Method
cpg	595.84	J/mol×K	974.24	Joback Method
dvisc	0.0008915	Pa×s	464.37	Joback Method

dvisc	0.0005213	Pa×s	512.89	Joback Method
dvisc	0.0003345	Pa×s	561.41	Joback Method
dvisc	0.0002303	Pa×s	609.93	Joback Method
dvisc	0.0001675	Pa×s	658.46	Joback Method
dvisc	0.0001273	Pa×s	706.98	Joback Method
dvisc	0.0001002	Pa×s	755.50	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=U356924&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