Phthalic acid, 2,2-dichloroethyl undecyl ester

Inchi: InChI=1S/C21H30Cl2O4/c1-2-3-4-5-6-7-8-9-12-15-26-20(24)17-13-10-11-14-18(17)21(25
InchiKey: QVHQHRHSVMLCEA-UHFFFAOYSA-N
Formula: C21H30Cl2O4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 417.37

Physical Properties

Property code	Value	Unit	Source
gf	-265.42	kJ/mol	Joback Method
hf	-778.07	kJ/mol	Joback Method
hfus	54.24	kJ/mol	Joback Method
hvap	91.97	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.335		Crippen Method
mcvol	322.350	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinpol	2822.00		NIST Webbook
rinpol	2822.00		NIST Webbook
tb	938.54	K	Joback Method
tc	1152.87	K	Joback Method
tf	554.53	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.93	J/mol×K	938.54	Joback Method
cpg	1047.93	J/mol×K	1117.15	Joback Method
cpg	1038.69	J/mol×K	1081.42	Joback Method
cpg	1028.30	J/mol×K	1045.70	Joback Method
cpg	1016.74	J/mol×K	1009.98	Joback Method
cpg	1003.96	J/mol×K	974.26	Joback Method
cpg	1056.06	J/mol×K	1152.87	Joback Method
dvisc	0.0000315	Pa×s	938.54	Joback Method

dvisc	0.0000411	Pa×s	874.54	Joback Method
dvisc	0.0000558	Pa×s	810.54	Joback Method
dvisc	0.0000798	Pa×s	746.53	Joback Method
dvisc	0.0001221	Pa×s	682.53	Joback Method
dvisc	0.0002040	Pa×s	618.53	Joback Method
dvisc	0.0003839	Pa×s	554.53	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=U356932&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