Sebacic acid, 2,2-dichloroethyl propyl ester

Inchi: InChI=1S/C15H26Cl2O4/c1-2-11-20-14(18)9-7-5-3-4-6-8-10-15(19)21-12-13(16)17/h13H
InchiKey: KPZNTXRWJPYAQO-UHFFFAOYSA-N
Formula: C15H26Cl2O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 341.27

Physical Properties

Property code	Value	Unit	Source
gf	-418.72	kJ/mol	Joback Method
hf	-879.29	kJ/mol	Joback Method
hfus	45.05	kJ/mol	Joback Method
hvap	75.68	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.407		Crippen Method
mcvol	261.570	ml/mol	McGowan Method
pc	1443.54	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	769.60	K	Joback Method
tc	957.30	K	Joback Method
tf	447.97	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.73	J/mol×K	769.60	Joback Method
cpg	802.08	J/mol×K	926.02	Joback Method
cpg	790.89	J/mol×K	894.74	Joback Method
cpg	778.87	J/mol×K	863.45	Joback Method
cpg	766.01	J/mol×K	832.17	Joback Method
cpg	752.30	J/mol×K	800.88	Joback Method
cpg	812.46	J/mol×K	957.30	Joback Method
dvisc	0.0000748	Pa×s	769.60	Joback Method

dvisc	0.0000986	Pa×s	715.99	Joback Method
dvisc	0.0001360	Pa×s	662.39	Joback Method
dvisc	0.0001983	Pa×s	608.78	Joback Method
dvisc	0.0003112	Pa×s	555.18	Joback Method
dvisc	0.0005376	Pa×s	501.57	Joback Method
dvisc	0.0010585	Pa×s	447.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355466&Units=SI
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

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