Sebacic acid, 2,2-dichloroethyl hexyl ester

Inchi: InChI=1S/C18H32Cl2O4/c1-2-3-4-11-14-23-17(21)12-9-7-5-6-8-10-13-18(22)24-15-16(19
InchiKey: QWXGZEQGDSGQHP-UHFFFAOYSA-N
Formula: C18H32Cl2O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 383.35

Physical Properties

Property code	Value	Unit	Source
gf	-393.46	kJ/mol	Joback Method
hf	-941.21	kJ/mol	Joback Method
hfus	52.82	kJ/mol	Joback Method
hvap	82.36	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.578		Crippen Method
mcvol	303.840	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	2542.00		NIST Webbook
tb	838.24	K	Joback Method
tc	1030.31	K	Joback Method
tf	481.78	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.10	J/mol×K	838.24	Joback Method
cpg	926.78	J/mol×K	870.25	Joback Method
cpg	941.44	J/mol×K	902.26	Joback Method
cpg	955.10	J/mol×K	934.28	Joback Method
cpg	967.78	J/mol×K	966.29	Joback Method
cpg	979.49	J/mol×K	998.30	Joback Method
cpg	990.25	J/mol×K	1030.31	Joback Method
dvisc	0.0007539	Pa×s	481.78	Joback Method
dvisc	0.0003701	Pa×s	541.19	Joback Method

dvisc	0.0002092	Pa×s	600.60	Joback Method
dvisc	0.0001310	Pa×s	660.01	Joback Method
dvisc	0.0000886	Pa×s	719.42	Joback Method
dvisc	0.0000637	Pa×s	778.83	Joback Method
dvisc	0.0000479	Pa×s	838.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355470&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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