Sebacic acid, 2,2-dichloroethyl nonyl ester

Inchi: InChI=1S/C21H38Cl2O4/c1-2-3-4-5-8-11-14-17-26-20(24)15-12-9-6-7-10-13-16-21(25)27
InchiKey: JMNNLXUXMDXZPN-UHFFFAOYSA-N
Formula: C21H38Cl2O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 425.43

Physical Properties

Property code	Value	Unit	Source
gf	-368.20	kJ/mol	Joback Method
hf	-1003.13	kJ/mol	Joback Method
hfus	60.59	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.748		Crippen Method
mcvol	346.110	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	2836.00		NIST Webbook
tb	906.88	K	Joback Method
tc	1110.28	K	Joback Method
tf	515.59	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1091.61	J/mol×K	906.88	Joback Method
cpg	1163.60	J/mol×K	1076.38	Joback Method
cpg	1151.56	J/mol×K	1042.48	Joback Method
cpg	1138.38	J/mol×K	1008.58	Joback Method
cpg	1124.01	J/mol×K	974.68	Joback Method
cpg	1108.43	J/mol×K	940.78	Joback Method
cpg	1174.51	J/mol×K	1110.28	Joback Method
dvisc	0.0000301	Pa×s	906.88	Joback Method
dvisc	0.0000403	Pa×s	841.66	Joback Method

dvisc	0.0000566	Pa×s	776.45	Joback Method
dvisc	0.0000847	Pa×s	711.23	Joback Method
dvisc	0.0001373	Pa×s	646.02	Joback Method
dvisc	0.0002481	Pa×s	580.80	Joback Method
dvisc	0.0005208	Pa×s	515.59	Joback Method

Sources

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=U355472&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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