Sebacic acid, 2,2-dichloroethyl undecyl ester

Inchi: InChI=1S/C23H42Cl2O4/c1-2-3-4-5-6-7-10-13-16-19-28-22(26)17-14-11-8-9-12-15-18-23
InchiKey: BQHLNJZKTOPKFN-UHFFFAOYSA-N
Formula: C23H42Cl2O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 453.48

Physical Properties

Property code	Value	Unit	Source
gf	-351.36	kJ/mol	Joback Method
hf	-1044.41	kJ/mol	Joback Method
hfus	65.77	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.528		Crippen Method
mcvol	374.290	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	952.64	K	Joback Method
tc	1168.33	K	Joback Method
tf	538.13	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.05	J/mol×K	952.64	Joback Method
cpg	1232.73	J/mol×K	988.59	Joback Method
cpg	1248.97	J/mol×K	1024.54	Joback Method
cpg	1263.80	J/mol×K	1060.49	Joback Method
cpg	1277.27	J/mol×K	1096.43	Joback Method
cpg	1289.41	J/mol×K	1132.38	Joback Method
cpg	1300.28	J/mol×K	1168.33	Joback Method
dvisc	0.0004012	Pa×s	538.13	Joback Method

dvisc	0.0001877	Pa×s	607.22	Joback Method
dvisc	0.0001026	Pa×s	676.30	Joback Method
dvisc	0.0000627	Pa×s	745.38	Joback Method
dvisc	0.0000416	Pa×s	814.47	Joback Method
dvisc	0.0000295	Pa×s	883.55	Joback Method
dvisc	0.0000220	Pa×s	952.64	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=U355474&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