Succinic acid, 2,2-dichloroethyl hexadecyl ester

Inchi: InChI=1S/C22H40Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-27-21(25)16-17-22(26

InchiKey: UOCYXFFWUUTHLW-UHFFFAOYSA-N

Formula: C22H40Cl2O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 439.46

Physical Properties

Property code	Value	Unit	Source
gf	-359.78	kJ/mol	Joback Method
hf	-1023.77	kJ/mol	Joback Method
hfus	63.18	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	7.138		Crippen Method
mcvol	360.200	ml/mol	McGowan Method
pc	916.05	kPa	Joback Method
rinpol	2909.00		NIST Webbook
rinpol	2909.00		NIST Webbook
tb	929.76	K	Joback Method
tc	1138.78	K	Joback Method
tf	526.86	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.06	J/mol×K	929.76	Joback Method
cpg	1226.23	J/mol×K	1103.94	Joback Method
cpg	1214.13	J/mol×K	1069.11	Joback Method
cpg	1200.80	J/mol×K	1034.27	Joback Method
cpg	1186.20	J/mol×K	999.43	Joback Method
cpg	1170.30	J/mol×K	964.60	Joback Method
cpg	1237.14	J/mol×K	1138.78	Joback Method
dvisc	0.0000257	Pa×s	929.76	Joback Method

dvisc	0.0000345	Pa×s	862.61	Joback Method
dvisc	0.0000486	Pa×s	795.46	Joback Method
dvisc	0.0000729	Pa×s	728.31	Joback Method
dvisc	0.0001188	Pa×s	661.16	Joback Method
dvisc	0.0002160	Pa×s	594.01	Joback Method
dvisc	0.0004577	Pa×s	526.86	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=U349415&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