Succinic acid, 2,2-dichloroethyl trans-4-methylcyclohexyl ester

Inchi: InChI=1S/C13H20Cl2O4/c1-9-2-4-10(5-3-9)19-13(17)7-6-12(16)18-8-11(14)15/h9-11H,2-

InchiKey: HAQDXGYIRCJKEB-UHFFFAOYSA-N

Formula: C13H20Cl2O4

SMILES: CC1CCC(OC(=O)CCC(=O)OCC(Cl)Cl)CC1

Mol. weight [g/mol]: 311.20

Physical Properties

Property code	Value	Unit	Source
gf	-418.82	kJ/mol	Joback Method
hf	-804.03	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	71.35	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.235		Crippen Method
mcvol	222.530	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	738.72	K	Joback Method
tc	951.12	K	Joback Method
tf	428.57	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.22	J/mol×K	738.72	Joback Method
cpg	639.15	J/mol×K	774.12	Joback Method
cpg	653.93	J/mol×K	809.52	Joback Method
cpg	667.57	J/mol×K	844.92	Joback Method
cpg	680.06	J/mol×K	880.32	Joback Method
cpg	691.40	J/mol×K	915.72	Joback Method
cpg	701.62	J/mol×K	951.12	Joback Method
dvisc	0.0015314	Pa×s	428.57	Joback Method

dvisc	0.0008116	Pa×s	480.26	Joback Method
dvisc	0.0004866	Pa×s	531.95	Joback Method
dvisc	0.0003194	Pa×s	583.64	Joback Method
dvisc	0.0002246	Pa×s	635.34	Joback Method
dvisc	0.0001665	Pa×s	687.03	Joback Method
dvisc	0.0001287	Pa×s	738.72	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=U390069&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