Succinic acid, 2,2-dichloroethyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C14H24Cl2O4/c1-10(7-14(2,3)4)8-19-12(17)5-6-13(18)20-9-11(15)16/h10-11H

InchiKey: BSRXMLQQEATODU-UHFFFAOYSA-N

Formula: C14H24Cl2O4

SMILES: CC(COC(=O)CCC(=O)OCC(Cl)Cl)CC(C)(C)C

Mol. weight [g/mol]: 327.24

Physical Properties

Property code	Value	Unit	Source
gf	-426.74	kJ/mol	Joback Method
hf	-872.68	kJ/mol	Joback Method
hfus	31.52	kJ/mol	Joback Method
hvap	71.77	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.729		Crippen Method
mcvol	247.480	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	743.05	K	Joback Method
tc	939.71	K	Joback Method
tf	424.12	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.57	J/mol×K	743.05	Joback Method
cpg	699.17	J/mol×K	775.83	Joback Method
cpg	712.85	J/mol×K	808.60	Joback Method
cpg	725.63	J/mol×K	841.38	Joback Method
cpg	737.55	J/mol×K	874.16	Joback Method
cpg	748.63	J/mol×K	906.93	Joback Method
cpg	758.90	J/mol×K	939.71	Joback Method
dvisc	0.0014003	Pa×s	424.12	Joback Method

dvisc	0.0006329	Pa×s	477.27	Joback Method
dvisc	0.0003354	Pa×s	530.43	Joback Method
dvisc	0.0001996	Pa×s	583.59	Joback Method
dvisc	0.0001295	Pa×s	636.74	Joback Method
dvisc	0.0000898	Pa×s	689.89	Joback Method
dvisc	0.0000656	Pa×s	743.05	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=U389542&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