Succinic acid, 2,2-dichloroethyl 3,3-dimethylbut-2-yl ester

Inchi: InChI=1S/C12H20Cl2O4/c1-8(12(2,3)4)18-11(16)6-5-10(15)17-7-9(13)14/h8-9H,5-7H2,1-

InchiKey: WABCDOCCPLWXER-UHFFFAOYSA-N

Formula: C12H20Cl2O4

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

Mol. weight [g/mol]: 299.19

Physical Properties

Property code	Value	Unit	Source
gf	-443.58	kJ/mol	Joback Method
hf	-831.40	kJ/mol	Joback Method
hfus	26.34	kJ/mol	Joback Method
hvap	67.32	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.091		Crippen Method
mcvol	219.300	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	697.29	K	Joback Method
tc	897.31	K	Joback Method
tf	401.58	K	Joback Method
vc	0.831	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.79	J/mol×K	697.29	Joback Method
cpg	590.59	J/mol×K	730.63	Joback Method
cpg	603.55	J/mol×K	763.96	Joback Method
cpg	615.66	J/mol×K	797.30	Joback Method
cpg	626.96	J/mol×K	830.64	Joback Method
cpg	637.47	J/mol×K	863.98	Joback Method
cpg	647.20	J/mol×K	897.31	Joback Method
dvisc	0.0017795	Pa×s	401.58	Joback Method

dvisc	0.0008223	Pa×s	450.87	Joback Method
dvisc	0.0004425	Pa×s	500.15	Joback Method
dvisc	0.0002661	Pa×s	549.43	Joback Method
dvisc	0.0001740	Pa×s	598.72	Joback Method
dvisc	0.0001214	Pa×s	648.00	Joback Method
dvisc	0.0000891	Pa×s	697.29	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U390621&Units=SI

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