Succinic acid, 3-methylbut-2-yl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H17Cl3O4/c1-7(2)8(3)18-10(16)5-4-9(15)17-6-11(12,13)14/h7-8H,4-6H2,1-

InchiKey: OGZAHCZVLHTAMY-UHFFFAOYSA-N

Formula: C11H17Cl3O4

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

Mol. weight [g/mol]: 319.61

Physical Properties

Property code	Value	Unit	Source
gf	-463.93	kJ/mol	Joback Method
hf	-826.50	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	69.47	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.268		Crippen Method
mcvol	217.450	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	711.84	K	Joback Method
tc	917.75	K	Joback Method
tf	420.23	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.10	J/mol×K	711.84	Joback Method
cpg	562.43	J/mol×K	746.16	Joback Method
cpg	573.93	J/mol×K	780.48	Joback Method
cpg	584.61	J/mol×K	814.79	Joback Method
cpg	594.51	J/mol×K	849.11	Joback Method
cpg	603.64	J/mol×K	883.43	Joback Method
cpg	612.03	J/mol×K	917.75	Joback Method
dvisc	0.0015182	Pa×s	420.23	Joback Method

dvisc	0.0007401	Pa×s	468.83	Joback Method
dvisc	0.0004129	Pa×s	517.43	Joback Method
dvisc	0.0002546	Pa×s	566.04	Joback Method
dvisc	0.0001695	Pa×s	614.64	Joback Method
dvisc	0.0001198	Pa×s	663.24	Joback Method
dvisc	0.0000887	Pa×s	711.84	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=U390230&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