Succinic acid, 3-methylbut-2-en-1-yl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C11H15Cl3O4/c1-8(2)5-6-17-9(15)3-4-10(16)18-7-11(12,13)14/h5H,3-4,6-7H2

InchiKey: QQCFQPGWUQZUAG-UHFFFAOYSA-N

Formula: C11H15Cl3O4

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

Mol. weight [g/mol]: 317.59

Physical Properties

Property code	Value	Unit	Source
gf	-387.38	kJ/mol	Joback Method
hf	-708.51	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	70.29	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.189		Crippen Method
mcvol	213.150	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tb	716.76	K	Joback Method
tc	925.75	K	Joback Method
tf	431.19	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.75	J/mol×K	716.76	Joback Method
cpg	536.16	J/mol×K	751.59	Joback Method
cpg	546.81	J/mol×K	786.42	Joback Method
cpg	556.72	J/mol×K	821.26	Joback Method
cpg	565.92	J/mol×K	856.09	Joback Method
cpg	574.46	J/mol×K	890.92	Joback Method
cpg	582.37	J/mol×K	925.75	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=U390232&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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