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

Inchi: InChI=1S/C12H19Cl3O4/c1-4-9(8(2)3)19-11(17)6-5-10(16)18-7-12(13,14)15/h8-9H,4-7H

InchiKey: BUBXDLJRIRMJOQ-UHFFFAOYSA-N

Formula: C12H19Cl3O4

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

Mol. weight [g/mol]: 333.64

Physical Properties

Property code	Value	Unit	Source
gf	-455.51	kJ/mol	Joback Method
hf	-847.14	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.658		Crippen Method
mcvol	231.540	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1835.00		NIST Webbook
rinpol	1835.00		NIST Webbook
tb	734.72	K	Joback Method
tc	938.40	K	Joback Method
tf	431.50	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.66	J/mol×K	734.72	Joback Method
cpg	615.44	J/mol×K	768.67	Joback Method
cpg	627.36	J/mol×K	802.61	Joback Method
cpg	638.44	J/mol×K	836.56	Joback Method
cpg	648.71	J/mol×K	870.51	Joback Method
cpg	658.18	J/mol×K	904.45	Joback Method
cpg	666.89	J/mol×K	938.40	Joback Method
dvisc	0.0013481	Pa×s	431.50	Joback Method

dvisc	0.0006492	Pa×s	482.04	Joback Method
dvisc	0.0003592	Pa×s	532.57	Joback Method
dvisc	0.0002202	Pa×s	583.11	Joback Method
dvisc	0.0001459	Pa×s	633.65	Joback Method
dvisc	0.0001028	Pa×s	684.18	Joback Method
dvisc	0.0000760	Pa×s	734.72	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=U390231&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