Succinic acid, 3-chlorophenyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H10Cl4O4/c13-8-2-1-3-9(6-8)20-11(18)5-4-10(17)19-7-12(14,15)16/h1-3,6

InchiKey: KFQSMSJBSUONIK-UHFFFAOYSA-N

Formula: C12H10Cl4O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 360.02

Physical Properties

Property code	Value	Unit	Source
gf	-359.78	kJ/mol	Joback Method
hf	-627.26	kJ/mol	Joback Method
hfus	35.44	kJ/mol	Joback Method
hvap	79.80	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.939		Crippen Method
mcvol	220.020	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	804.69	K	Joback Method
tc	1039.21	K	Joback Method
tf	530.36	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.94	J/mol×K	804.69	Joback Method
cpg	566.46	J/mol×K	1000.12	Joback Method
cpg	560.64	J/mol×K	961.04	Joback Method
cpg	554.02	J/mol×K	921.95	Joback Method
cpg	546.56	J/mol×K	882.86	Joback Method
cpg	538.21	J/mol×K	843.78	Joback Method
cpg	571.51	J/mol×K	1039.21	Joback Method
dvisc	0.0000760	Pa×s	804.69	Joback Method

dvisc	0.0000958	Pa×s	758.97	Joback Method
dvisc	0.0001243	Pa×s	713.25	Joback Method
dvisc	0.0001672	Pa×s	667.53	Joback Method
dvisc	0.0002348	Pa×s	621.80	Joback Method
dvisc	0.0003482	Pa×s	576.08	Joback Method
dvisc	0.0005524	Pa×s	530.36	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=U390239&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