Succinic acid, 4-chloro-3-methylphenyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C13H12Cl4O4/c1-8-6-9(2-3-10(8)14)21-12(19)5-4-11(18)20-7-13(15,16)17/h2-

InchiKey: IOHWGWJPXZJPAK-UHFFFAOYSA-N

Formula: C13H12Cl4O4

SMILES: Cc1cc(OC(=O)CCC(=O)OCC(Cl)(Cl)Cl)ccc1Cl

Mol. weight [g/mol]: 374.04

Physical Properties

Property code	Value	Unit	Source
gf	-360.99	kJ/mol	Joback Method
hf	-659.37	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.247		Crippen Method
mcvol	234.110	ml/mol	McGowan Method
pc	2062.36	kPa	Joback Method
rinpol	2420.00		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	832.55	K	Joback Method
tc	1064.31	K	Joback Method
tf	554.15	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.86	J/mol×K	832.55	Joback Method
cpg	589.49	J/mol×K	871.18	Joback Method
cpg	598.17	J/mol×K	909.80	Joback Method
cpg	605.95	J/mol×K	948.43	Joback Method
cpg	612.87	J/mol×K	987.05	Joback Method
cpg	618.94	J/mol×K	1025.68	Joback Method
cpg	624.21	J/mol×K	1064.31	Joback Method
dvisc	0.0004349	Pa×s	554.15	Joback Method

dvisc	0.0002812	Pa×s	600.55	Joback Method
dvisc	0.0001936	Pa×s	646.95	Joback Method
dvisc	0.0001401	Pa×s	693.35	Joback Method
dvisc	0.0001055	Pa×s	739.75	Joback Method
dvisc	0.0000822	Pa×s	786.15	Joback Method
dvisc	0.0000659	Pa×s	832.55	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=U390241&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