Succinic acid, 2,4,6-trichlorophenyl 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C12H8Cl6O4/c13-6-3-7(14)11(8(15)4-6)22-10(20)2-1-9(19)21-5-12(16,17)18/h

InchiKey: GNXCORFQNNSESA-UHFFFAOYSA-N

Formula: C12H8Cl6O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(Cl)(Cl)Cl

Mol. weight [g/mol]: 428.91

Physical Properties

Property code	Value	Unit	Source
gf	-402.90	kJ/mol	Joback Method
hf	-681.68	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	89.89	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.246		Crippen Method
mcvol	244.500	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
rinpol	2543.00		NIST Webbook
tb	889.51	K	Joback Method
tc	1130.38	K	Joback Method
tf	615.24	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.94	J/mol×K	889.51	Joback Method
cpg	566.86	J/mol×K	929.66	Joback Method
cpg	572.91	J/mol×K	969.80	Joback Method
cpg	578.12	J/mol×K	1009.95	Joback Method
cpg	582.53	J/mol×K	1050.09	Joback Method
cpg	586.16	J/mol×K	1090.24	Joback Method
cpg	589.06	J/mol×K	1130.38	Joback Method
dvisc	0.0002921	Pa×s	615.24	Joback Method
dvisc	0.0002010	Pa×s	660.95	Joback Method

dvisc	0.0001452	Pa×s	706.66	Joback Method
dvisc	0.0001091	Pa×s	752.38	Joback Method
dvisc	0.0000847	Pa×s	798.09	Joback Method
dvisc	0.0000676	Pa×s	843.80	Joback Method
dvisc	0.0000552	Pa×s	889.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390244&Units=SI
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

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