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

Inchi: InChI=1S/C12H11Cl3O4/c13-8-2-1-3-9(6-8)19-12(17)5-4-11(16)18-7-10(14)15/h1-3,6,10
InchiKey: FFKWHAMGQPJLMF-UHFFFAOYSA-N
Formula: C12H11Cl3O4
SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1)OCC(Cl)Cl
Mol. weight [g/mol]: 325.57

Physical Properties

Property code	Value	Unit	Source
gf	-353.13	kJ/mol	Joback Method
hf	-608.05	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.372		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	770.05	K	Joback Method
tc	994.90	K	Joback Method
tf	483.02	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.15	J/mol×K	770.05	Joback Method
cpg	517.61	J/mol×K	807.52	Joback Method
cpg	527.16	J/mol×K	845.00	Joback Method
cpg	535.82	J/mol×K	882.47	Joback Method
cpg	543.58	J/mol×K	919.95	Joback Method
cpg	550.47	J/mol×K	957.42	Joback Method
cpg	556.49	J/mol×K	994.90	Joback Method
dvisc	0.0008152	Pa×s	483.02	Joback Method

dvisc	0.0004916	Pa×s	530.86	Joback Method
dvisc	0.0003223	Pa×s	578.70	Joback Method
dvisc	0.0002254	Pa×s	626.54	Joback Method
dvisc	0.0001658	Pa×s	674.37	Joback Method
dvisc	0.0001271	Pa×s	722.21	Joback Method
dvisc	0.0001006	Pa×s	770.05	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=U389852&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