Succinic acid, ethyl 2,3,6-trichlorophenyl ester

Inchi: InChI=1S/C12H11Cl3O4/c1-2-18-9(16)5-6-10(17)19-12-8(14)4-3-7(13)11(12)15/h3-4H,2,
InchiKey: VQAWDMHUBWVGEG-UHFFFAOYSA-N
Formula: C12H11Cl3O4
SMILES: CCOC(=O)CCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 325.57

Physical Properties

Property code	Value	Unit	Source
gf	-369.95	kJ/mol	Joback Method
hf	-625.71	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	78.03	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.896		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	780.45	K	Joback Method
tc	1003.15	K	Joback Method
tf	523.06	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.14	J/mol×K	780.45	Joback Method
cpg	513.26	J/mol×K	817.57	Joback Method
cpg	522.53	J/mol×K	854.68	Joback Method
cpg	530.96	J/mol×K	891.80	Joback Method
cpg	538.53	J/mol×K	928.92	Joback Method
cpg	545.24	J/mol×K	966.04	Joback Method
cpg	551.09	J/mol×K	1003.15	Joback Method
dvisc	0.0005598	Pa×s	523.06	Joback Method

dvisc	0.0003857	Pa×s	565.96	Joback Method
dvisc	0.0002801	Pa×s	608.86	Joback Method
dvisc	0.0002121	Pa×s	651.75	Joback Method
dvisc	0.0001663	Pa×s	694.65	Joback Method
dvisc	0.0001341	Pa×s	737.55	Joback Method
dvisc	0.0001107	Pa×s	780.45	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=U349701&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