Succinic acid, 2,4,6-trichlorophenyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C18H15Cl3O4/c1-10-4-3-5-15(11(10)2)24-16(22)6-7-17(23)25-18-13(20)8-12(

InchiKey: YSIQDBTTXRILSO-UHFFFAOYSA-N

Formula: C18H15Cl3O4

SMILES: Cc1cccc(OC(=O)CCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1C

Mol. weight [g/mol]: 401.67

Physical Properties

Property code	Value	Unit	Source
gf	-226.28	kJ/mol	Joback Method
hf	-535.96	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	94.99	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.555		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	954.37	K	Joback Method
tc	1194.80	K	Joback Method
tf	642.14	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.96	J/mol×K	954.37	Joback Method
cpg	734.36	J/mol×K	994.44	Joback Method
cpg	742.48	J/mol×K	1034.51	Joback Method
cpg	749.34	J/mol×K	1074.58	Joback Method
cpg	754.93	J/mol×K	1114.66	Joback Method
cpg	759.28	J/mol×K	1154.73	Joback Method
cpg	762.40	J/mol×K	1194.80	Joback Method
dvisc	0.0002468	Pa×s	642.14	Joback Method

dvisc	0.0001725	Pa×s	694.18	Joback Method
dvisc	0.0001268	Pa×s	746.22	Joback Method
dvisc	0.0000970	Pa×s	798.26	Joback Method
dvisc	0.0000767	Pa×s	850.29	Joback Method
dvisc	0.0000623	Pa×s	902.33	Joback Method
dvisc	0.0000517	Pa×s	954.37	Joback Method

Sources

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=U390031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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