Succinic acid, 2,4,6-trichlorophenyl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C18H15Cl3O5/c1-10-3-4-14(24-2)15(7-10)25-16(22)5-6-17(23)26-18-12(20)8-1

InchiKey: VNNONIAJJJYMBN-UHFFFAOYSA-N

Formula: C18H15Cl3O5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 417.67

Physical Properties

Property code	Value	Unit	Source
gf	-331.28	kJ/mol	Joback Method
hf	-668.18	kJ/mol	Joback Method
hfus	47.87	kJ/mol	Joback Method
hvap	97.40	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.255		Crippen Method
mcvol	274.430	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	976.79	K	Joback Method
tc	1216.43	K	Joback Method
tf	664.37	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.98	J/mol×K	976.79	Joback Method
cpg	757.43	J/mol×K	1016.73	Joback Method
cpg	764.43	J/mol×K	1056.67	Joback Method
cpg	769.98	J/mol×K	1096.61	Joback Method
cpg	774.06	J/mol×K	1136.55	Joback Method
cpg	776.68	J/mol×K	1176.49	Joback Method
cpg	777.80	J/mol×K	1216.43	Joback Method
dvisc	0.0001787	Pa×s	664.37	Joback Method

dvisc	0.0001260	Pa×s	716.44	Joback Method
dvisc	0.0000932	Pa×s	768.51	Joback Method
dvisc	0.0000717	Pa×s	820.58	Joback Method
dvisc	0.0000568	Pa×s	872.65	Joback Method
dvisc	0.0000463	Pa×s	924.72	Joback Method
dvisc	0.0000385	Pa×s	976.79	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=U390968&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