Succinic acid, 3,4-dimethylphenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C18H16Cl2O4/c1-11-6-7-13(10-12(11)2)23-16(21)8-9-17(22)24-15-5-3-4-14(19

InchiKey: LSFREGXRBBDROE-UHFFFAOYSA-N

Formula: C18H16Cl2O4

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)cc1C

Mol. weight [g/mol]: 367.22

Physical Properties

Property code	Value	Unit	Source
gf	-204.72	kJ/mol	Joback Method
hf	-508.75	kJ/mol	Joback Method
hfus	42.87	kJ/mol	Joback Method
hvap	89.94	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.901		Crippen Method
mcvol	256.320	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2886.00		NIST Webbook
tb	911.96	K	Joback Method
tc	1148.51	K	Joback Method
tf	599.70	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.74	J/mol×K	911.96	Joback Method
cpg	718.63	J/mol×K	951.39	Joback Method
cpg	728.26	J/mol×K	990.81	Joback Method
cpg	736.66	J/mol×K	1030.24	Joback Method
cpg	743.84	J/mol×K	1069.66	Joback Method
cpg	749.81	J/mol×K	1109.09	Joback Method
cpg	754.59	J/mol×K	1148.51	Joback Method
dvisc	0.0003162	Pa×s	599.70	Joback Method
dvisc	0.0002136	Pa×s	651.74	Joback Method

dvisc	0.0001529	Pa×s	703.79	Joback Method
dvisc	0.0001146	Pa×s	755.83	Joback Method
dvisc	0.0000892	Pa×s	807.87	Joback Method
dvisc	0.0000715	Pa×s	859.92	Joback Method
dvisc	0.0000588	Pa×s	911.96	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=U357568&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