Succinic acid, 2,4,6-trichlorophenyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H12Cl4O5/c1-24-14-8-9(18)2-3-13(14)25-15(22)4-5-16(23)26-17-11(20)6-1

InchiKey: YDWDFIWSBQWUPT-UHFFFAOYSA-N

Formula: C17H12Cl4O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 438.09

Physical Properties

Property code	Value	Unit	Source
gf	-351.63	kJ/mol	Joback Method
hf	-663.28	kJ/mol	Joback Method
hfus	49.47	kJ/mol	Joback Method
hvap	99.56	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.600		Crippen Method
mcvol	272.580	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	3068.00		NIST Webbook
rinpol	3068.00		NIST Webbook
tb	991.34	K	Joback Method
tc	1235.87	K	Joback Method
tf	683.02	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.15	J/mol×K	991.34	Joback Method
cpg	716.07	J/mol×K	1032.09	Joback Method
cpg	721.56	J/mol×K	1072.85	Joback Method
cpg	725.61	J/mol×K	1113.60	Joback Method
cpg	728.22	J/mol×K	1154.36	Joback Method
cpg	729.37	J/mol×K	1195.11	Joback Method
cpg	729.04	J/mol×K	1235.87	Joback Method
dvisc	0.0001674	Pa×s	683.02	Joback Method

dvisc	0.0001198	Pa×s	734.41	Joback Method
dvisc	0.0000895	Pa×s	785.79	Joback Method
dvisc	0.0000694	Pa×s	837.18	Joback Method
dvisc	0.0000554	Pa×s	888.57	Joback Method
dvisc	0.0000453	Pa×s	939.95	Joback Method
dvisc	0.0000378	Pa×s	991.34	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=U390945&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