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

Inchi: InChI=1S/C17H13Cl3O5/c1-23-13-4-2-3-5-14(13)24-15(21)6-7-16(22)25-17-11(19)8-10(1

InchiKey: ITQZEGHCMOJCDQ-UHFFFAOYSA-N

Formula: C17H13Cl3O5

SMILES: COc1ccccc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 403.64

Physical Properties

Property code	Value	Unit	Source
gf	-330.07	kJ/mol	Joback Method
hf	-636.07	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	94.51	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.947		Crippen Method
mcvol	260.340	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2871.00		NIST Webbook
rinpol	2871.00		NIST Webbook
tb	948.93	K	Joback Method
tc	1189.37	K	Joback Method
tf	640.58	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.87	J/mol×K	948.93	Joback Method
cpg	723.88	J/mol×K	1149.29	Joback Method
cpg	720.83	J/mol×K	1109.22	Joback Method
cpg	716.39	J/mol×K	1069.15	Joback Method
cpg	710.58	J/mol×K	1029.08	Joback Method
cpg	703.41	J/mol×K	989.00	Joback Method
cpg	725.56	J/mol×K	1189.37	Joback Method
dvisc	0.0000435	Pa×s	948.93	Joback Method

dvisc	0.0000525	Pa×s	897.54	Joback Method
dvisc	0.0000650	Pa×s	846.15	Joback Method
dvisc	0.0000827	Pa×s	794.76	Joback Method
dvisc	0.0001087	Pa×s	743.36	Joback Method
dvisc	0.0001488	Pa×s	691.97	Joback Method
dvisc	0.0002143	Pa×s	640.58	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=U389718&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