Succinic acid, di(4-chloro-2-methoxyphenyl) ester

Inchi: InChI=1S/C18H16Cl2O6/c1-23-15-9-11(19)3-5-13(15)25-17(21)7-8-18(22)26-14-6-4-12(2

InchiKey: ZSCOVYXMQHWNEH-UHFFFAOYSA-N

Formula: C18H16Cl2O6

SMILES: COc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

Mol. weight [g/mol]: 399.22

Physical Properties

Property code	Value	Unit	Source
gf	-414.72	kJ/mol	Joback Method
hf	-773.19	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	94.76	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.302		Crippen Method
mcvol	268.060	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	3021.00		NIST Webbook
rinpol	3021.00		NIST Webbook
tb	956.80	K	Joback Method
tc	1191.46	K	Joback Method
tf	644.16	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.32	J/mol×K	956.80	Joback Method
cpg	787.42	J/mol×K	1152.35	Joback Method
cpg	784.57	J/mol×K	1113.24	Joback Method
cpg	780.11	J/mol×K	1074.13	Joback Method
cpg	774.07	J/mol×K	1035.02	Joback Method
cpg	766.46	J/mol×K	995.91	Joback Method
cpg	788.64	J/mol×K	1191.46	Joback Method
dvisc	0.0000328	Pa×s	956.80	Joback Method

dvisc	0.0000397	Pa×s	904.69	Joback Method
dvisc	0.0000493	Pa×s	852.59	Joback Method
dvisc	0.0000629	Pa×s	800.48	Joback Method
dvisc	0.0000830	Pa×s	748.37	Joback Method
dvisc	0.0001141	Pa×s	696.27	Joback Method
dvisc	0.0001653	Pa×s	644.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390949&Units=SI
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

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