Succinic acid, 4-chloro-3-methylphenyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C18H16BrClO5/c1-11-9-13(4-5-14(11)20)24-17(21)7-8-18(22)25-15-6-3-12(19)

InchiKey: LKQDVPUELRSKTC-UHFFFAOYSA-N

Formula: C18H16BrClO5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 427.67

Physical Properties

Property code	Value	Unit	Source
gf	-283.47	kJ/mol	Joback Method
hf	-598.90	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	94.40	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.711		Crippen Method
mcvol	267.450	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	963.11	K	Joback Method
tc	1204.54	K	Joback Method
tf	651.81	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.92	J/mol×K	963.11	Joback Method
cpg	750.37	J/mol×K	1003.35	Joback Method
cpg	758.43	J/mol×K	1043.59	Joback Method
cpg	765.12	J/mol×K	1083.83	Joback Method
cpg	770.45	J/mol×K	1124.06	Joback Method
cpg	774.41	J/mol×K	1164.30	Joback Method
cpg	777.02	J/mol×K	1204.54	Joback Method
dvisc	0.0001939	Pa×s	651.81	Joback Method

dvisc	0.0001353	Pa×s	703.69	Joback Method
dvisc	0.0000992	Pa×s	755.58	Joback Method
dvisc	0.0000757	Pa×s	807.46	Joback Method
dvisc	0.0000597	Pa×s	859.34	Joback Method
dvisc	0.0000483	Pa×s	911.23	Joback Method
dvisc	0.0000400	Pa×s	963.11	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=U390922&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