Succinic acid, 3-chlorophenyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C17H14BrClO5/c1-22-15-9-11(18)5-6-14(15)24-17(21)8-7-16(20)23-13-4-2-3-1

InchiKey: FVVWPENVVJYCDT-UHFFFAOYSA-N

Formula: C17H14BrClO5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 413.65

Physical Properties

Property code	Value	Unit	Source
gf	-282.26	kJ/mol	Joback Method
hf	-566.79	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	91.52	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.402		Crippen Method
mcvol	253.360	ml/mol	McGowan Method
pc	2212.45	kPa	Joback Method
rinpol	2914.00		NIST Webbook
rinpol	2914.00		NIST Webbook
tb	935.25	K	Joback Method
tc	1178.11	K	Joback Method
tf	628.02	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.54	J/mol×K	935.25	Joback Method
cpg	696.03	J/mol×K	975.73	Joback Method
cpg	704.20	J/mol×K	1016.20	Joback Method
cpg	711.06	J/mol×K	1056.68	Joback Method
cpg	716.63	J/mol×K	1097.16	Joback Method
cpg	720.92	J/mol×K	1137.64	Joback Method
cpg	723.94	J/mol×K	1178.11	Joback Method
dvisc	0.0002341	Pa×s	628.02	Joback Method

dvisc	0.0001606	Pa×s	679.23	Joback Method
dvisc	0.0001162	Pa×s	730.43	Joback Method
dvisc	0.0000877	Pa×s	781.63	Joback Method
dvisc	0.0000685	Pa×s	832.84	Joback Method
dvisc	0.0000550	Pa×s	884.05	Joback Method
dvisc	0.0000453	Pa×s	935.25	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U390921&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