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

Inchi: InChI=1S/C17H13BrCl2O5/c1-23-14-9-10(18)5-6-12(14)24-15(21)7-8-16(22)25-13-4-2-3-

InchiKey: LDYUMWWEXYIKKQ-UHFFFAOYSA-N

Formula: C17H13BrCl2O5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 448.09

Physical Properties

Property code	Value	Unit	Source
gf	-303.82	kJ/mol	Joback Method
hf	-594.00	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.056		Crippen Method
mcvol	265.600	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	977.66	K	Joback Method
tc	1224.20	K	Joback Method
tf	670.46	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.83	J/mol×K	977.66	Joback Method
cpg	709.76	J/mol×K	1018.75	Joback Method
cpg	716.34	J/mol×K	1059.84	Joback Method
cpg	721.57	J/mol×K	1100.93	Joback Method
cpg	725.46	J/mol×K	1142.02	Joback Method
cpg	728.02	J/mol×K	1183.11	Joback Method
cpg	729.24	J/mol×K	1224.20	Joback Method
dvisc	0.0001810	Pa×s	670.46	Joback Method

dvisc	0.0001282	Pa×s	721.66	Joback Method
dvisc	0.0000950	Pa×s	772.86	Joback Method
dvisc	0.0000731	Pa×s	824.06	Joback Method
dvisc	0.0000580	Pa×s	875.26	Joback Method
dvisc	0.0000472	Pa×s	926.46	Joback Method
dvisc	0.0000393	Pa×s	977.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390923&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