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

Inchi: InChI=1S/C17H12BrCl3O5/c1-24-14-6-9(18)2-3-13(14)25-15(22)4-5-16(23)26-17-11(20)

InchiKey: AFVHWYWUXHUNOK-UHFFFAOYSA-N

Formula: C17H12BrCl3O5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 482.54

Physical Properties

Property code	Value	Unit	Source
gf	-325.38	kJ/mol	Joback Method
hf	-621.21	kJ/mol	Joback Method
hfus	50.56	kJ/mol	Joback Method
hvap	101.61	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	5.709		Crippen Method
mcvol	277.840	ml/mol	McGowan Method
pc	2010.90	kPa	Joback Method
rinpol	3182.00		NIST Webbook
rinpol	3182.00		NIST Webbook
tb	1020.07	K	Joback Method
tc	1270.62	K	Joback Method
tf	712.90	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.08	J/mol×K	1020.07	Joback Method
cpg	732.65	J/mol×K	1228.86	Joback Method
cpg	731.95	J/mol×K	1187.10	Joback Method
cpg	729.84	J/mol×K	1145.35	Joback Method
cpg	726.33	J/mol×K	1103.59	Joback Method
cpg	721.41	J/mol×K	1061.83	Joback Method
cpg	731.94	J/mol×K	1270.62	Joback Method
dvisc	0.0000339	Pa×s	1020.07	Joback Method

dvisc	0.0000404	Pa×s	968.88	Joback Method
dvisc	0.0000491	Pa×s	917.68	Joback Method
dvisc	0.0000610	Pa×s	866.49	Joback Method
dvisc	0.0000780	Pa×s	815.29	Joback Method
dvisc	0.0001029	Pa×s	764.10	Joback Method
dvisc	0.0001414	Pa×s	712.90	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=U390925&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