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

Inchi: InChI=1S/C17H13BrClFO4/c1-10-8-12(3-4-14(10)19)23-16(21)6-7-17(22)24-15-5-2-11(2

InchiKey: WIBQJAOJFTZDPY-UHFFFAOYSA-N

Formula: C17H13BrClFO4

SMILES: Cc1cc(OC(=O)CCC(=O)Oc2ccc(F)cc2Br)ccc1Cl

Mol. weight [g/mol]: 415.64

Physical Properties

Property code	Value	Unit	Source
gf	-381.70	kJ/mol	Joback Method
hf	-642.15	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	88.95	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.841		Crippen Method
mcvol	249.260	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	917.08	K	Joback Method
tc	1155.05	K	Joback Method
tf	618.90	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.57	J/mol×K	917.08	Joback Method
cpg	677.30	J/mol×K	956.74	Joback Method
cpg	685.89	J/mol×K	996.40	Joback Method
cpg	693.36	J/mol×K	1036.06	Joback Method
cpg	699.75	J/mol×K	1075.73	Joback Method
cpg	705.07	J/mol×K	1115.39	Joback Method
cpg	709.35	J/mol×K	1155.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389773&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
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