Succinic acid, 2-bromo-4-fluorophenyl 3,4-dimethylphenyl ester

Inchi: InChI=1S/C18H16BrFO4/c1-11-3-5-14(9-12(11)2)23-17(21)7-8-18(22)24-16-6-4-13(20)10

InchiKey: ZSPACVMSJPGHFR-UHFFFAOYSA-N

Formula: C18H16BrFO4

SMILES: Cc1ccc(OC(=O)CCC(=O)Oc2ccc(F)cc2Br)cc1C

Mol. weight [g/mol]: 395.22

Physical Properties

Property code	Value	Unit	Source
gf	-361.35	kJ/mol	Joback Method
hf	-647.05	kJ/mol	Joback Method
hfus	42.84	kJ/mol	Joback Method
hvap	86.79	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.496		Crippen Method
mcvol	251.110	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	2712.00		NIST Webbook
rinpol	2712.00		NIST Webbook
tb	902.53	K	Joback Method
tc	1135.19	K	Joback Method
tf	600.25	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.97	J/mol×K	902.53	Joback Method
cpg	715.18	J/mol×K	941.31	Joback Method
cpg	725.22	J/mol×K	980.08	Joback Method
cpg	734.11	J/mol×K	1018.86	Joback Method
cpg	741.87	J/mol×K	1057.63	Joback Method
cpg	748.53	J/mol×K	1096.41	Joback Method
cpg	754.11	J/mol×K	1135.19	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=U358017&Units=SI

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