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

Inchi: InChI=1S/C16H11BrF2O4/c17-13-9-11(19)4-5-14(13)23-16(21)7-6-15(20)22-12-3-1-2-10

InchiKey: IDNKLJXQJRUYKO-UHFFFAOYSA-N

Formula: C16H11BrF2O4

SMILES: O=C(CCC(=O)Oc1ccc(F)cc1Br)Oc1cccc(F)c1

Mol. weight [g/mol]: 385.16

Physical Properties

Property code	Value	Unit	Source
gf	-563.37	kJ/mol	Joback Method
hf	-790.41	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	80.86	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.019		Crippen Method
mcvol	224.700	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	851.06	K	Joback Method
tc	1080.48	K	Joback Method
tf	565.78	K	Joback Method
vc	0.862	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.28	J/mol×K	851.06	Joback Method
cpg	612.65	J/mol×K	889.30	Joback Method
cpg	621.97	J/mol×K	927.53	Joback Method
cpg	630.28	J/mol×K	965.77	Joback Method
cpg	637.58	J/mol×K	1004.01	Joback Method
cpg	643.91	J/mol×K	1042.24	Joback Method
cpg	649.30	J/mol×K	1080.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358015&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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