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

Inchi: InChI=1S/C16H10BrCl2FO4/c17-10-8-9(20)4-5-12(10)23-14(21)6-7-15(22)24-13-3-1-2-1

InchiKey: SMDJVDWZNSTZIG-UHFFFAOYSA-N

Formula: C16H10BrCl2FO4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccc(F)cc1Br

Mol. weight [g/mol]: 436.06

Physical Properties

Property code	Value	Unit	Source
gf	-402.05	kJ/mol	Joback Method
hf	-637.25	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	91.11	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.186		Crippen Method
mcvol	247.410	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	2831.00		NIST Webbook
rinpol	2831.00		NIST Webbook
tb	931.63	K	Joback Method
tc	1175.00	K	Joback Method
tf	637.55	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.05	J/mol×K	931.63	Joback Method
cpg	638.28	J/mol×K	972.19	Joback Method
cpg	645.42	J/mol×K	1012.75	Joback Method
cpg	651.48	J/mol×K	1053.32	Joback Method
cpg	656.50	J/mol×K	1093.88	Joback Method
cpg	660.49	J/mol×K	1134.44	Joback Method
cpg	663.49	J/mol×K	1175.00	Joback Method

Sources

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=U358018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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