Succinic acid, 8-chlorooctyl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C18H23BrClFO4/c19-15-13-14(21)7-8-16(15)25-18(23)10-9-17(22)24-12-6-4-2

InchiKey: GYBPCKHETDYPQM-UHFFFAOYSA-N

Formula: C18H23BrClFO4

SMILES: O=C(CCC(=O)Oc1ccc(F)cc1Br)OCCCCCCCCCl

Mol. weight [g/mol]: 437.73

Physical Properties

Property code	Value	Unit	Source
gf	-466.43	kJ/mol	Joback Method
hf	-876.38	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	87.58	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.396		Crippen Method
mcvol	287.110	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2840.00		NIST Webbook
rinpol	2840.00		NIST Webbook
tb	903.32	K	Joback Method
tc	1114.98	K	Joback Method
tf	578.71	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.23	J/mol×K	903.32	Joback Method
cpg	843.66	J/mol×K	938.60	Joback Method
cpg	855.04	J/mol×K	973.87	Joback Method
cpg	865.40	J/mol×K	1009.15	Joback Method
cpg	874.77	J/mol×K	1044.43	Joback Method
cpg	883.17	J/mol×K	1079.71	Joback Method
cpg	890.62	J/mol×K	1114.98	Joback Method

Sources

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=U389775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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