Succinic acid, 2-chloro-6-fluorophenyl 1-bromo-3,3,3-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H10BrClF4O4/c14-6-9(13(17,18)19)22-10(20)4-5-11(21)23-12-7(15)2-1-3-8

InchiKey: PNFSSEMKWPUOHO-UHFFFAOYSA-N

Formula: C13H10BrClF4O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 421.57

Physical Properties

Property code	Value	Unit	Source
gf	-1092.56	kJ/mol	Joback Method
hf	-1375.54	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.034		Crippen Method
mcvol	221.970	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	783.06	K	Joback Method
tc	988.67	K	Joback Method
tf	511.55	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.29	J/mol×K	783.06	Joback Method
cpg	589.00	J/mol×K	817.33	Joback Method
cpg	597.91	J/mol×K	851.60	Joback Method
cpg	606.06	J/mol×K	885.87	Joback Method
cpg	613.47	J/mol×K	920.14	Joback Method
cpg	620.18	J/mol×K	954.40	Joback Method
cpg	626.22	J/mol×K	988.67	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=U390829&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