Succinic acid, 1,1,1-trifluoroprop-2-yl 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C13H11BrF4O4/c1-7(13(16,17)18)21-11(19)4-5-12(20)22-10-3-2-8(15)6-9(10)1

InchiKey: SCADHSSELGOOAG-UHFFFAOYSA-N

Formula: C13H11BrF4O4

SMILES: CC(OC(=O)CCC(=O)Oc1ccc(F)cc1Br)C(F)(F)F

Mol. weight [g/mol]: 387.12

Physical Properties

Property code	Value	Unit	Source
gf	-1080.63	kJ/mol	Joback Method
hf	-1359.80	kJ/mol	Joback Method
hfus	34.93	kJ/mol	Joback Method
hvap	67.93	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.768		Crippen Method
mcvol	209.730	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
rinpol	1747.00		NIST Webbook
rinpol	1747.00		NIST Webbook
tb	745.63	K	Joback Method
tc	947.46	K	Joback Method
tf	481.63	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.41	J/mol×K	745.63	Joback Method
cpg	568.12	J/mol×K	779.27	Joback Method
cpg	578.03	J/mol×K	812.91	Joback Method
cpg	587.17	J/mol×K	846.54	Joback Method
cpg	595.56	J/mol×K	880.18	Joback Method
cpg	603.24	J/mol×K	913.82	Joback Method
cpg	610.22	J/mol×K	947.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389761&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