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

Inchi: InChI=1S/C13H11BrF4O4/c14-7-10(13(16,17)18)22-12(20)6-5-11(19)21-9-4-2-1-3-8(9)15

InchiKey: KKHXVKPYKIDVFL-UHFFFAOYSA-N

Formula: C13H11BrF4O4

SMILES: O=C(CCC(=O)OC(CBr)C(F)(F)F)Oc1ccccc1F

Mol. weight [g/mol]: 387.12

Physical Properties

Property code	Value	Unit	Source
gf	-1071.00	kJ/mol	Joback Method
hf	-1348.33	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	67.27	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.380		Crippen Method
mcvol	209.730	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	740.65	K	Joback Method
tc	941.67	K	Joback Method
tf	469.11	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.85	J/mol×K	740.65	Joback Method
cpg	569.67	J/mol×K	774.15	Joback Method
cpg	579.67	J/mol×K	807.66	Joback Method
cpg	588.88	J/mol×K	841.16	Joback Method
cpg	597.34	J/mol×K	874.66	Joback Method
cpg	605.07	J/mol×K	908.16	Joback Method
cpg	612.12	J/mol×K	941.67	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=U390826&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