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

Inchi: InChI=1S/C14H14BrF3O5/c1-8(14(16,17)18)22-12(19)5-6-13(20)23-10-4-3-9(15)7-11(10

InchiKey: RCFPWYLMWCRPQU-UHFFFAOYSA-N

Formula: C14H14BrF3O5

SMILES: COc1cc(Br)ccc1OC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 399.16

Physical Properties

Property code	Value	Unit	Source
gf	-982.40	kJ/mol	Joback Method
hf	-1316.55	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.637		Crippen Method
mcvol	227.920	ml/mol	McGowan Method
pc	2019.95	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	791.66	K	Joback Method
tc	997.77	K	Joback Method
tf	514.54	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.90	J/mol×K	791.66	Joback Method
cpg	639.20	J/mol×K	826.01	Joback Method
cpg	649.58	J/mol×K	860.36	Joback Method
cpg	659.08	J/mol×K	894.72	Joback Method
cpg	667.70	J/mol×K	929.07	Joback Method
cpg	675.47	J/mol×K	963.42	Joback Method
cpg	682.40	J/mol×K	997.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390909&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

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