Succinic acid, 2,2,3,3-tetrafluoropropyl 4-bromo-2-methoxyphenyl ester

Inchi: InChI=1S/C14H13BrF4O5/c1-22-10-6-8(15)2-3-9(10)24-12(21)5-4-11(20)23-7-14(18,19)

InchiKey: CATBKQOXSGOVLV-UHFFFAOYSA-N

Formula: C14H13BrF4O5

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

Mol. weight [g/mol]: 417.15

Physical Properties

Property code	Value	Unit	Source
gf	-1177.21	kJ/mol	Joback Method
hf	-1512.66	kJ/mol	Joback Method
hfus	38.71	kJ/mol	Joback Method
hvap	72.56	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.587		Crippen Method
mcvol	229.690	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	2135.00		NIST Webbook
rinpol	2135.00		NIST Webbook
tb	790.93	K	Joback Method
tc	991.09	K	Joback Method
tf	515.13	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.57	J/mol×K	790.93	Joback Method
cpg	646.45	J/mol×K	824.29	Joback Method
cpg	656.46	J/mol×K	857.65	Joback Method
cpg	665.63	J/mol×K	891.01	Joback Method
cpg	673.96	J/mol×K	924.37	Joback Method
cpg	681.49	J/mol×K	957.73	Joback Method
cpg	688.23	J/mol×K	991.09	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=U390910&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