Succinic acid, 1,1,1-trifluoroprop-2-yl 3-methoxyphenyl ester

Inchi: InChI=1S/C14H15F3O5/c1-9(14(15,16)17)21-12(18)6-7-13(19)22-11-5-3-4-10(8-11)20-2

InchiKey: SSJVXYHCGLKIMS-UHFFFAOYSA-N

Formula: C14H15F3O5

SMILES: COc1cccc(OC(=O)CCC(=O)OC(C)C(F)(F)F)c1

Mol. weight [g/mol]: 320.26

Physical Properties

Property code	Value	Unit	Source
gf	-987.09	kJ/mol	Joback Method
hf	-1331.41	kJ/mol	Joback Method
hfus	30.73	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.875		Crippen Method
mcvol	210.420	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	720.52	K	Joback Method
tc	915.39	K	Joback Method
tf	442.22	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.23	J/mol×K	720.52	Joback Method
cpg	606.18	J/mol×K	753.00	Joback Method
cpg	618.24	J/mol×K	785.48	Joback Method
cpg	629.44	J/mol×K	817.95	Joback Method
cpg	639.79	J/mol×K	850.43	Joback Method
cpg	649.30	J/mol×K	882.91	Joback Method
cpg	657.98	J/mol×K	915.39	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=U390973&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