Succinic acid, 1,1,1-trifluoroprop-2-yl 2-methoxy-5-methylphenyl ester

Inchi: InChI=1S/C15H17F3O5/c1-9-4-5-11(21-3)12(8-9)23-14(20)7-6-13(19)22-10(2)15(16,17)1

InchiKey: GFMUKDUKGXXXHL-UHFFFAOYSA-N

Formula: C15H17F3O5

SMILES: COc1ccc(C)cc1OC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 334.29

Physical Properties

Property code	Value	Unit	Source
gf	-988.30	kJ/mol	Joback Method
hf	-1363.52	kJ/mol	Joback Method
hfus	32.93	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.183		Crippen Method
mcvol	224.510	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	748.38	K	Joback Method
tc	942.93	K	Joback Method
tf	466.01	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.99	J/mol×K	748.38	Joback Method
cpg	659.20	J/mol×K	780.81	Joback Method
cpg	671.51	J/mol×K	813.23	Joback Method
cpg	682.93	J/mol×K	845.66	Joback Method
cpg	693.46	J/mol×K	878.08	Joback Method
cpg	703.12	J/mol×K	910.51	Joback Method
cpg	711.92	J/mol×K	942.93	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=U390950&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