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

Inchi: InChI=1S/C14H13F5O5/c1-22-10-6-8(15)2-3-9(10)24-12(21)5-4-11(20)23-7-14(18,19)13

InchiKey: BSLZZSZETTZZDG-UHFFFAOYSA-N

Formula: C14H13F5O5

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

Mol. weight [g/mol]: 356.24

Physical Properties

Property code	Value	Unit	Source
gf	-1386.34	kJ/mol	Joback Method
hf	-1735.10	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	65.31	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.963		Crippen Method
mcvol	213.960	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1847.00		NIST Webbook
rinpol	1847.00		NIST Webbook
tb	724.04	K	Joback Method
tc	907.97	K	Joback Method
tf	455.92	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.90	J/mol×K	724.04	Joback Method
cpg	619.82	J/mol×K	754.69	Joback Method
cpg	630.95	J/mol×K	785.35	Joback Method
cpg	641.32	J/mol×K	816.00	Joback Method
cpg	650.93	J/mol×K	846.66	Joback Method
cpg	659.79	J/mol×K	877.31	Joback Method
cpg	667.90	J/mol×K	907.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390895&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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