Succinic acid, 1,1,1-trifluoroprop-2-yl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C14H11F7O4/c1-7(13(16,17)18)24-10(22)5-6-11(23)25-9-4-2-3-8(12(9)15)14(1

InchiKey: XELNBIQJRSDBDV-UHFFFAOYSA-N

Formula: C14H11F7O4

SMILES: CC(OC(=O)CCC(=O)Oc1cccc(C(F)(F)F)c1F)C(F)(F)F

Mol. weight [g/mol]: 376.22

Physical Properties

Property code	Value	Unit	Source
gf	-1668.12	kJ/mol	Joback Method
hf	-2003.85	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	59.97	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.024		Crippen Method
mcvol	211.630	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1565.00		NIST Webbook
rinpol	1565.00		NIST Webbook
tb	696.93	K	Joback Method
tc	876.10	K	Joback Method
tf	437.29	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.48	J/mol×K	696.93	Joback Method
cpg	611.96	J/mol×K	726.79	Joback Method
cpg	622.67	J/mol×K	756.65	Joback Method
cpg	632.64	J/mol×K	786.52	Joback Method
cpg	641.90	J/mol×K	816.38	Joback Method
cpg	650.48	J/mol×K	846.24	Joback Method
cpg	658.41	J/mol×K	876.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390776&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