Succinic acid, 1,1,1-trifluoroprop-2-yl pentafluorobenzyl ester

Inchi: InChI=1S/C14H10F8O4/c1-5(14(20,21)22)26-8(24)3-2-7(23)25-4-6-9(15)11(17)13(19)12

InchiKey: COIOXBKUZJWVQL-UHFFFAOYSA-N

Formula: C14H10F8O4

SMILES: CC(OC(=O)CCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(F)(F)F

Mol. weight [g/mol]: 394.21

Physical Properties

Property code	Value	Unit	Source
gf	-1894.66	kJ/mol	Joback Method
hf	-2225.62	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	62.44	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.699		Crippen Method
mcvol	213.400	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1573.00		NIST Webbook
rinpol	1573.00		NIST Webbook
tb	714.37	K	Joback Method
tc	886.42	K	Joback Method
tf	473.02	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.33	J/mol×K	714.37	Joback Method
cpg	613.00	J/mol×K	743.04	Joback Method
cpg	623.05	J/mol×K	771.72	Joback Method
cpg	632.48	J/mol×K	800.39	Joback Method
cpg	641.30	J/mol×K	829.07	Joback Method
cpg	649.51	J/mol×K	857.74	Joback Method
cpg	657.11	J/mol×K	886.42	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=U389876&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