Succinic acid, 2-fluorophenyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C13H10F6O4/c14-8-3-1-2-4-9(8)23-11(21)6-5-10(20)22-7-12(15,16)13(17,18)1

InchiKey: AQDHILROBPIWRI-UHFFFAOYSA-N

Formula: C13H10F6O4

SMILES: O=C(CCC(=O)Oc1ccccc1F)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 344.21

Physical Properties

Property code	Value	Unit	Source
gf	-1469.66	kJ/mol	Joback Method
hf	-1770.35	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	58.29	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.252		Crippen Method
mcvol	195.770	ml/mol	McGowan Method
pc	1906.90	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	670.24	K	Joback Method
tc	852.45	K	Joback Method
tf	427.91	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.58	J/mol×K	670.24	Joback Method
cpg	552.99	J/mol×K	700.61	Joback Method
cpg	563.61	J/mol×K	730.98	Joback Method
cpg	573.49	J/mol×K	761.35	Joback Method
cpg	582.66	J/mol×K	791.71	Joback Method
cpg	591.14	J/mol×K	822.08	Joback Method
cpg	598.97	J/mol×K	852.45	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=U390867&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

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