Succinic acid, 2-fluorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C14H11F7O4/c15-8-3-1-2-4-9(8)25-11(23)6-5-10(22)24-7-13(17,18)12(16)14(1

InchiKey: HVVQJZUQJXCHIM-UHFFFAOYSA-N

Formula: C14H11F7O4

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

Mol. weight [g/mol]: 376.22

Physical Properties

Property code	Value	Unit	Source
gf	-1658.49	kJ/mol	Joback Method
hf	-1992.38	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	59.31	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.590		Crippen Method
mcvol	211.630	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1662.00		NIST Webbook
tb	691.95	K	Joback Method
tc	870.26	K	Joback Method
tf	424.77	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.50	J/mol×K	691.95	Joback Method
cpg	613.12	J/mol×K	721.67	Joback Method
cpg	623.95	J/mol×K	751.39	Joback Method
cpg	634.02	J/mol×K	781.10	Joback Method
cpg	643.36	J/mol×K	810.82	Joback Method
cpg	652.02	J/mol×K	840.54	Joback Method
cpg	660.01	J/mol×K	870.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390804&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