Succinic acid, 3,5-difluorophenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C14H9F9O4/c15-7-3-8(16)5-9(4-7)27-11(25)2-1-10(24)26-6-12(17,18)13(19,20

InchiKey: IWLJFDSOJKLONE-UHFFFAOYSA-N

Formula: C14H9F9O4

SMILES: O=C(CCC(=O)Oc1cc(F)cc(F)c1)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 412.20

Physical Properties

Property code	Value	Unit	Source
gf	-2052.46	kJ/mol	Joback Method
hf	-2399.54	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.026		Crippen Method
mcvol	215.170	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	1546.00		NIST Webbook
rinpol	1546.00		NIST Webbook
tb	692.68	K	Joback Method
tc	865.59	K	Joback Method
tf	455.89	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.71	J/mol×K	692.68	Joback Method
cpg	629.45	J/mol×K	721.50	Joback Method
cpg	639.44	J/mol×K	750.32	Joback Method
cpg	648.71	J/mol×K	779.13	Joback Method
cpg	657.30	J/mol×K	807.95	Joback Method
cpg	665.25	J/mol×K	836.77	Joback Method
cpg	672.60	J/mol×K	865.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358030&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