Succinic acid, 2,2,3,3-tetrafluoropropyl 3-nitrophenyl ester

Inchi: InChI=1S/C13H11F4NO6/c14-12(15)13(16,17)7-23-10(19)4-5-11(20)24-9-3-1-2-8(6-9)18

InchiKey: USGNPGKRSUIIRH-UHFFFAOYSA-N

Formula: C13H11F4NO6

SMILES: O=C(CCC(=O)Oc1cccc([N+](=O)[O-])c1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 353.22

Physical Properties

Property code	Value	Unit	Source
gf	-1049.77	kJ/mol	Joback Method
hf	-1385.42	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	77.42	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.724		Crippen Method
mcvol	209.650	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2121.00		NIST Webbook
tb	826.33	K	Joback Method
tc	1037.86	K	Joback Method
tf	552.92	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.89	J/mol×K	826.33	Joback Method
cpg	629.78	J/mol×K	861.59	Joback Method
cpg	638.74	J/mol×K	896.84	Joback Method
cpg	646.82	J/mol×K	932.10	Joback Method
cpg	654.04	J/mol×K	967.35	Joback Method
cpg	660.45	J/mol×K	1002.61	Joback Method
cpg	666.07	J/mol×K	1037.86	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=U390132&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