Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-nitrophenyl ester

Inchi: InChI=1S/C15H11F8NO6/c16-12(17)14(20,21)15(22,23)13(18,19)7-29-10(25)4-5-11(26)
InchiKey: BOFQALYLHLDHMZ-UHFFFAOYSA-N
Formula: C15H11F8NO6
SMILES: O=C(CCC(=O)Oc1cccc([N+](=O)[O-])c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 453.24

Physical Properties

Property code	Value	Unit	Source
gf	-1806.49	kJ/mol	Joback Method
hf	-2228.64	kJ/mol	Joback Method
hfus	44.07	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.995		Crippen Method
mcvol	244.910	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
rinpol	2190.00		NIST Webbook
tb	862.71	K	Joback Method
tc	1065.80	K	Joback Method
tf	582.66	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.83	J/mol×K	862.71	Joback Method
cpg	771.06	J/mol×K	896.56	Joback Method
cpg	779.45	J/mol×K	930.41	Joback Method
cpg	787.09	J/mol×K	964.26	Joback Method
cpg	794.03	J/mol×K	998.11	Joback Method
cpg	800.37	J/mol×K	1031.96	Joback Method
cpg	806.17	J/mol×K	1065.80	Joback Method

Sources

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=U390133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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