2-Nitro-3,4,6-trifluoroacetanilide

Inchi: InChI=1S/C8H5F3N2O3/c1-3(14)12-7-5(10)2-4(9)6(11)8(7)13(15)16/h2H,1H3,(H,12,14)
InchiKey: CAJSFXVPIMWHPO-UHFFFAOYSA-N
Formula: C8H5F3N2O3
SMILES: CC(=O)Nc1c(F)cc(F)c(F)c1[N+](=O)[O-]
Mol. weight [g/mol]: 234.13
CAS: 388-11-4

Physical Properties

Property code	Value	Unit	Source
gf	-498.04	kJ/mol	Joback Method
hf	-676.00	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	65.65	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	1.970		Crippen Method
mcvol	134.100	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	682.73	K	Joback Method
tc	901.68	K	Joback Method
tf	504.39	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.40	J/mol×K	682.73	Joback Method
cpg	347.98	J/mol×K	719.22	Joback Method
cpg	355.96	J/mol×K	755.71	Joback Method
cpg	363.34	J/mol×K	792.21	Joback Method
cpg	370.14	J/mol×K	828.70	Joback Method
cpg	376.37	J/mol×K	865.19	Joback Method
cpg	382.05	J/mol×K	901.68	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=C388114&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume