Acetamide, N-(3-nitrophenyl)-2,2,2-trifluoro-

Inchi: InChI=1S/C8H5F3N2O3/c9-8(10,11)7(14)12-5-2-1-3-6(4-5)13(15)16/h1-4H,(H,12,14)
InchiKey: ODXWGMFPJCIUCW-UHFFFAOYSA-N
Formula: C8H5F3N2O3
SMILES: O=C(Nc1cccc([N+](=O)[O-])c1)C(F)(F)F
Mol. weight [g/mol]: 234.13

Physical Properties

Property code	Value	Unit	Source
gf	-466.31	kJ/mol	Joback Method
hf	-650.34	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	62.37	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.096		Crippen Method
mcvol	134.100	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1522.00		NIST Webbook
tb	664.56	K	Joback Method
tc	893.27	K	Joback Method
tf	469.25	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.06	J/mol×K	664.56	Joback Method
cpg	357.34	J/mol×K	702.68	Joback Method
cpg	365.76	J/mol×K	740.80	Joback Method
cpg	373.38	J/mol×K	778.92	Joback Method
cpg	380.28	J/mol×K	817.04	Joback Method
cpg	386.52	J/mol×K	855.15	Joback Method
cpg	392.15	J/mol×K	893.27	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=U307314&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