Methanamine, 1,1,1-trifluoro-N-[2,2,2-trifluoro-1-(trifluoromethyl)

Other names: Methylamine, 1,1,1-trifluoro-N-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]-
Methylamine, trifluoro-N-[trifluoro-1-(trifluoromethyl)ethylidene]-
1,1,1-Trifluoro-N-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]-methanamine

Inchi: InChI=1S/C4F9N/c5-2(6,7)1(3(8,9)10)14-4(11,12)13

InchiKey: NPHAEKPPAZLGTQ-UHFFFAOYSA-N

Formula: C4F9N

SMILES: FC(F)(F)N=C(C(F)(F)F)C(F)(F)F

Mol. weight [g/mol]: 233.04

CAS: 453-22-5

Physical Properties

Property code	Value	Unit	Source
hf	-1844.70	kJ/mol	Joback Method
hvap	16.65	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.072		Crippen Method
mcvol	88.830	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
tb	351.22	K	Joback Method
tc	493.99	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	22.20	kJ/mol	288.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C453225&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

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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