1H-Pyrazole, 3-methyl-5-(trifluoromethyl)-

Other names:	Pyrazole, 3-methyl-5-(trifluoromethyl)-
	Pyrazole, 3(or 5)-methyl-5(or 3)-(trifluoromethyl)-
	3-Methyl-5-(trifluoromethyl)pyrazole
	3(5)-Trifluoromethyl-5(3)-methylpyrazole
Inchi:	InChI=1S/C5H5F3N2/c1-3-2-4(10-9-3)5(6,7)8/h2H,1H3,(H,9,10)
InchiKey:	DLCHCAYDSKIFIN-UHFFFAOYSA-N
Formula:	C5H5F3N2
SMILES:	Cc1cc(C(F)(F)F)[nH]n1
Mol. weight [g/mol]:	150.10
CAS:	10010-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.255		Crippen Method
mcvol	87.120	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	78.20 ± 0.80	kJ/mol	297.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10010932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume