

Purine, 2-(trifluoromethyl)-

Inchi:	InChI=1S/C6H3F3N4/c7-6(8,9)5-10-1-3-4(13-5)12-2-11-3/h1-2H,(H,10,11,12,13)
InchiKey:	YDAGLPIQWWSUJT-UHFFFAOYSA-N
Formula:	C6H3F3N4
SMILES:	FC(F)(F)c1ncc2ncnc-2[nH]1
Mol. weight [g/mol]:	188.11
CAS:	95121-04-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	0.841		Crippen Method
mcvol	101.710	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C95121043&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/96-786-4/Purine-2-trifluoromethyl.pdf>

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