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