Purine, 6-(2,2,2-trifluoroethylthio)-

Inchi:	InChI=1S/C7H5F3N4S/c8-7(9,10)1-15-6-4-5(12-2-11-4)13-3-14-6/h2-3H,1H2,(H,11,12,13
InchiKey:	KFNWKYCGNGQQEN-UHFFFAOYSA-N
Formula:	C7H5F3N4S
SMILES:	FC(F)(F)CSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	234.20
CAS:	654-18-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	1.525		Crippen Method
mcvol	132.150	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=C654182&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:
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