

Purine, 6-(2,2,2-trifluoroethoxy)-

Inchi:	InChI=1S/C7H5F3N4O/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:	DIWYLTCCAAMWNB-UHFFFAOYSA-N
Formula:	C7H5F3N4O
SMILES:	FC(F)(F)COc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	218.14
CAS:	73972-56-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	0.812		Crippen Method
mcvol	121.670	ml/mol	McGowan Method

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=C73972562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/26-291-0/Purine-6-2-2-2-trifluoroethoxy.pdf>

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