

Adenine, N4-trifluoroacetyl-

Inchi:	InChI=1S/C7H4F3N5O/c8-7(9,10)6(16)15-5-3-4(12-1-11-3)13-2-14-5/h1-2H,(H2,11,12,13)
InchiKey:	AKNFGGUYIWQHAN-UHFFFAOYSA-N
Formula:	C7H4F3N5O
SMILES:	O=C(Nc1ncnc2[nH]cnc12)C(F)(F)F
Mol. weight [g/mol]:	231.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.66		Crippen Method
logp	0.372		Crippen Method
mcvol	127.350	ml/mol	McGowan Method
rinpol	1740.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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