

N-(5-Methylisoxazol-3-yl)-N-(trifluoroacetyl)-2,2,2-

Other names:	3-Bis(trifluoroacetyl)amino-5-methylisoxazole Isoxazole, 3-bis(trifluoroacetyl)amino-5-methyl- 5-Methylisoxazol-3-bis(trifluoroacetyl)amine 5-Methylisoxazol-3-amine bis(trifluoroacetate)
Inchi:	InChI=1S/C8H4F6N2O3/c1-3-2-4(15-19-3)16(5(17)7(9,10)11)6(18)8(12,13)14/h2H,1H3
InchiKey:	NAMGGXJNKGJNCI-UHFFFAOYSA-N
Formula:	C8H4F6N2O3
SMILES:	<chem>Cc1cc(N(C(=O)C(F)(F)F)C(=O)C(F)(F)F)no1</chem>
Mol. weight [g/mol]:	290.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.07		Crippen Method
logp	1.967		Crippen Method
mcvol	143.710	ml/mol	McGowan Method
rinpol	964.00		NIST Webbook
rinpol	964.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373356&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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