

N-Trifluoroacetylmorpholine

Other names:	Trifluoroacetic acid, morpholide
Inchi:	InChI=1S/C6H8F3NO2/c7-6(8,9)5(11)10-1-3-12-4-2-10/h1-4H2
InchiKey:	UTPCRKXZUFAUIB-UHFFFAOYSA-N
Formula:	C6H8F3NO2
SMILES:	O=C(N1CCOCC1)C(F)(F)F
Mol. weight [g/mol]:	183.13
CAS:	360-95-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.32		Crippen Method
logp	0.408		Crippen Method
mcvol	107.270	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C360952&Units=SI

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/63-927-3/N-Trifluoroacetylmorpholine.pdf>

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