

Trifluoroacetic acid, morpholide

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

Physical Properties

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

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C360952&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/63-927-3/Trifluoroacetic-acid-morpholide.pdf>

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