

4-Methyl-5-trifluoromethyl-4H-1,2,4-triazolin-3(2H)-thione

Other names:	3H-1,2,4-Triazole-3-thione, 2,4-dihydro-4-methyl-5-(trifluoromethyl)-2,4-dihydro-4-methyl-5-(trifluoromethyl)-3H-1,2,4-triazole-3-thione
Inchi:	InChI=1S/C4H4F3N3S/c1-10-2(4(5,6)7)8-9-3(10)11/h1H3,(H,9,11)
InchiKey:	HUZASKHMPBJXJP-UHFFFAOYSA-N
Formula:	C4H4F3N3S
SMILES:	Cn1c(S)nnc1C(F)(F)F
Mol. weight [g/mol]:	183.16
CAS:	30682-81-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	1.123		Crippen Method
mcvol	99.360	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30682816&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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