

2-Amino-5-trifluoromethyl-1,3,4-thiadiazole

Other names:	1,3,4-Thiadiazol-2-amine, 5-(trifluoromethyl)- 1,3,4-Thiadiazole, 2-amino-5-(trifluoromethyl)- 2-Amino-5-trifluoromethyl-1,3,4-triazole 5-Trifluoromethyl-[1,3,4]thiadiazol-2-ylamine
Inchi:	InChI=1S/C3H2F3N3S/c4-3(5,6)1-8-9-2(7)10-1/h(H2,7,9)
InchiKey:	LTEUXHSAYOSFGQ-UHFFFAOYSA-N
Formula:	C3H2F3N3S
SMILES:	<chem>Nc1nnc(C(F)(F)F)s1</chem>
Mol. weight [g/mol]:	169.13
CAS:	10444-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.139		Crippen Method
mcvol	85.270	ml/mol	McGowan Method

Sources

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=C10444890&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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