

2-Amino-5-tert-butyl-1,3,4-thiadiazole

Other names:	1,3,4-Thiadiazol-2-amine, 5-(1,1-dimethylethyl)- 5-tert-butyl-1,3,4-thiadiazol-2-amine
Inchi:	InChI=1S/C6H11N3S/c1-6(2,3)4-8-9-5(7)10-4/h1-3H3,(H2,7,9)
InchiKey:	ICXDPEFCLDSXLI-UHFFFAOYSA-N
Formula:	C6H11N3S
SMILES:	CC(C)(C)c1n[nH]c(=N)s1
Mol. weight [g/mol]:	157.24
CAS:	39222-73-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	0.766		Crippen Method
mcvol	122.230	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=C39222736&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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