

4-t-Butylurazole

Other names:	4-tert-Butylurazole 1,2,4-Triazolidine-3,5-dione, 4-(1,1-dimethylethyl)- 4-tert-butyl-1,2,4-triazolidine-3,5-dione
Inchi:	InChI=1S/C6H11N3O2/c1-6(2,3)9-4(10)7-8-5(9)11/h1-3H3,(H,7,10)(H,8,11)
InchiKey:	OYNMWNWYHCJZHL-UHFFFAOYSA-N
Formula:	C6H11N3O2
SMILES:	CC(C)(C)n1c(=O)[nH][nH]c1=O
Mol. weight [g/mol]:	157.17
CAS:	35403-67-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.47		Crippen Method
logp	-1.344		Crippen Method
mcvol	117.620	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C35403679&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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