

1,2,4-Triazin-5(4H)-one, 6-(1,1-dimethylethyl)-4-[(2-methylpropylidene)amino]

Other names:	Isomethiozin 6-tert-butyl-4-isobutylidenamino-3-methylthio-1,2,4-triazin-5-one
Inchi:	InChI=1S/C12H20N4OS/c1-8(2)7-13-16-10(17)9(12(3,4)5)14-15-11(16)18-6/h7-8H,1-6H
InchiKey:	MZTLOILRKLUURT-UHFFFAOYSA-N
Formula:	C12H20N4OS
SMILES:	CSc1nnc(C(C)(C)C)c(=O)n1N=CC(C)C
Mol. weight [g/mol]:	268.38
CAS:	57052-04-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	2.148		Crippen Method
mcvol	214.020	ml/mol	McGowan Method
rinpol	1948.00		NIST Webbook
rinpol	1953.00		NIST Webbook

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=C57052047&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
rinpol:	Non-polar retention indices

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