Isomethiozin

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,1-6H3
InchiKey:	MZTLOILRKLUURT-UHFFFAOYSA-N
Formula:	C12H20N4OS
SMILES:	CSc1nnc(C(C)(C)C)c(=O)n1N=CC(C)C
Mol. weight [g/mol]:	268.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Cheméo Relay (1.0)
logp	2.148		Crippen Method
mcvol	214.020	ml/mol	McGowan Method
rinpol	1948.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tf	365.05	K	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57052047&Units=SI

Legend

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

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point