Pymetrozin

Other names:	(E)-4,5-dihydro-6-methyl-4-(3-pyridinylmethyleneamino)-1,2,4-triazin-3(2H)-one 1,2,4-Triazin-3(2H)-one, 4,5-dihydro-6-methyl-4-[(E)-(3-pyridinylmethylene)amino]- 4,5-dihydro-6-methyl-4-[(E)-(3-pyridinylmethylene)amino]-1,2,4-triazin-3(2H)-one pymetrozine
Inchi:	InChI=1S/C10H11N5O/c1-8-7-15(10(16)14-13-8)12-6-9-3-2-4-11-5-9/h2-6H,7H2,1H3,(H,
InchiKey:	QHMTXANCGGJZRX-UHFFFAOYSA-N
Formula:	C10H11N5O
SMILES:	CC1=NNC(=O)N(N=Cc2cccnc2)C1
Mol. weight [g/mol]:	217.23
CAS:	123312-89-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	0.817		Crippen Method
mcvol	160.010	ml/mol	McGowan Method
rinpol	2235.30		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility Determination and Model Correlation of Pymetrozine and Evaluation of the Effect of Solvent Properties and Composition:	https://www.doi.org/10.1021/acs.jced.9b00229
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123312890&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