

FENAMIDONE

Other names: 4H-Imidazol-4-one,
3,5-dihydro-5-methyl-2-(methylthio)-5-phenyl-3-(phenylamino)- (5S)-
(S)-3,5-dihydro-5-methyl-2-(methylthio)-5-phenyl-3-(phenylamino)-4H-imidazol-4-one

Inchi: InChI=1S/C17H17N3OS/c1-17(13-9-5-3-6-10-13)15(21)20(16(18-17)22-2)19-14-11-7-4-8

InchiKey: LMVPQMGRYSRMIW-UHFFFAOYSA-N

Formula: C17H17N3OS

SMILES: CSC1=NC(C)(c2ccccc2)C(=O)N1Nc1ccccc1

Mol. weight [g/mol]: 311.40

CAS: 161326-34-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.21		Crippen Method
logp	3.490		Crippen Method
mcvol	235.570	ml/mol	McGowan Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C161326347&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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