Morazone

Other names:	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-4-[(3-methyl-2-phenyl-4-morpholinyl)methyl]-2-phenyl-
	Antipyrine, 4-((3-methyl-2-phenylmorpholino)methyl)-
	Novartrina
	Orsimon
	R 445
	Tarugan
	3-Pyrazolin-5-one, 2,3-dimethyl-4-(3-methyl-2-phenylmorpholino)methyl-1-phenyl-
	4-(2'-Phenyl-3'-methylmorpholinomethyl)-1-phenyl-2,3-dimethyl-3-pyrazoline-5-one
	4-((3-Methyl-2-phenylmorpholino)methyl)antipyrine
	4-[(3-Methyl-2-phenyl-4-morpholino)methyl]antipyrine
	NSC 292156
Inchi:	InChI=1S/C23H27N3O2/c1-17-21(23(27)26(24(17)3)20-12-8-5-9-13-20)16-25-14-15-28-2
InchiKey:	OOGNFQMTGRZRAB-UHFFFAOYSA-N
Formula:	C23H27N3O2
SMILES:	Cc1c(CN2CCOC(c3ccccc3)C2C)c(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]:	377.48
CAS:	6536-18-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	3.446		Crippen Method
mcvol	298.770	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=C6536181&Units=SI

Legend

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