

Famprofazone

Other names:	3H-Pyrazol-3-one, 1,2-dihydro-1-methyl-4-(1-methylethyl)-5-[[methyl(1-methyl-2-phenylethyl)amino]methyl]-2-pyrazolin-5-one, Pyrazolin-5-one, 4-isopropyl-2-methyl-1-phenyl-3-((1-phenyl-2-propyl)methylamino)methyl-antipyrine, Antipyrine, 4-isopropyl-3-(«alpha»-(methyl-(1-phenyl-2-propyl)amino))-3-(N-Methyl-(«alpha»-methyl-«beta»-phenyl)-ethyl-aminomethyl)-4-isopropyl-norantipyrin 4-Isopropyl-2-methyl-3-([methyl(«alpha»-methylphenethyl)amino]methyl)-1-phenyl-3-pyrazolin-5-one 3-(N,«alpha»-Dimethylphenethylaminomethyl)-4-isopropyl-2-methyl-1-phenyl-3-pyrazolin-5-one
Inchi:	InChI=1S/C24H31N3O/c1-18(2)23-22(17-25(4)19(3)16-20-12-8-6-9-13-20)26(5)27(24(23
InchiKey:	GNUXVOXXWGNPIV-UHFFFAOYSA-N
Formula:	C24H31N3O
SMILES:	<chem>CC(C)c1c(CN(C)C(C)Cc2ccccc2)n(C)n(-c2ccccc2)c1=O</chem>
Mol. weight [g/mol]:	377.52
CAS:	22881-35-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	4.362		Crippen Method
mcvol	317.850	ml/mol	McGowan Method
rinpol	3059.00		NIST Webbook
rinpol	3059.00		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=C22881352&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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