Acetamide, N-antipyrinyl-

Other names:	Acetamide, N-(2,3-dihydro-1,5-dimethyl-3-oxo-2-phenyl-1H-pyrazol-4-yl)-
	Acetamidoantipyrine
	Acetyl-4-aminoantipyrine
	Acetylaminoantipyrine
	Acetylated 4-aminoantipyrine
	Antipyrine, 4-acetamido-
	N-Acetyl-4-aminoantipyrine
	4-Acetamidoantipyrine
	4-Acetaminoantipyrine
	4-Acetoaminoantipyrine
	4-Acetylaminoantipyrine
	4-Acetylaminophenazone
	Aminoantipyrine, N-acetyl-
	4-(N-Acetylamino)antipyrine
	NSC 331807
	N-(2,3-dimethyl-5-oxo-1-phenyl-3-pyrazolin-4-yl)acetamide
Inchi:	InChI=1S/C13H15N3O2/c1-9-12(14-10(2)17)13(18)16(15(9)3)11-7-5-4-6-8-11/h4-8H,1-3
InchiKey:	OIAGWXKSCXPNNZ-UHFFFAOYSA-N
Formula:	C13H15N3O2
SMILES:	CC(=O)Nc1c(C)n(C)n(-c2ccccc2)c1=O
Mol. weight [g/mol]:	245.28
CAS:	83-15-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	1.443		Crippen Method
mcvol	188.190	ml/mol	McGowan Method
rinpol	2278.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83158&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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