Propyphenazone

Other names:	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-4-(1-methylethyl)-2-phenyl- Antipyrine, 4-isopropyl- 2,3-Dimethyl-4-isopropyl-1-phenyl-3H-pyrazolin-5-one Isopropylantipyrin Isopropylantipyrine 4-Isopropylantipyrine 4-Isopropyl-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one Isopropylphenazone Larodon 1-Phenyl-2,3-dimethyl-4-isopropyl-3-pyrazolin-5-one 1-Phenyl-2,3-dimethyl-4-isopropylpyrazol-5-one 3-Pyrazolin-5-one, 2,3-dimethyl-4-isopropyl-1-phenyl- 3-Pyrazolin-5-one, 4-isopropyl-2,3-dimethyl-1-phenyl- Isopropyrine 4-Isopropylphenazone Budirol Causyth Cibalgina Eufibron Isopropchin
Inchi:	InChI=1S/C14H18N2O/c1-10(2)13-11(3)15(4)16(14(13)17)12-8-6-5-7-9-12/h5-10H,1-4H3
InchiKey:	PXWLVJLKJGVOKE-UHFFFAOYSA-N
Formula:	C14H18N2O
SMILES:	Cc1c(C(C)C)c(=O)n(-c2ccccc2)n1C
Mol. weight [g/mol]:	230.31
CAS:	479-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	2.608		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1925.00		NIST Webbook
rinpol	1917.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1917.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C479925&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices