

2-Pyrazoline, 5-ethyl-3,5-dimethyl, 1-benzoyl

Inchi:	InChI=1S/C14H18N2O/c1-4-14(3)10-11(2)15-16(14)13(17)12-8-6-5-7-9-12/h5-9H,4,10H2
InchiKey:	SBXDTMIOGHVNGJ-UHFFFAOYSA-N
Formula:	C14H18N2O
SMILES:	CCC1(C)CC(C)=NN1C(=O)c1ccccc1
Mol. weight [g/mol]:	230.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.87		Crippen Method
logp	3.077		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpola	1789.00		NIST Webbook
rinpola	1789.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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