

2-Pyrazoline, 4,4-dimethyl-5-(1-methylethyl), 1-benzoyl

Inchi:	InChI=1S/C15H20N2O/c1-11(2)13-15(3,4)10-16-17(13)14(18)12-8-6-5-7-9-12/h5-11,13H
InchiKey:	VSDNWFKINBKURY-UHFFFAOYSA-N
Formula:	C15H20N2O
SMILES:	CC(C)C1N(C(=O)c2ccccc2)N=CC1(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.179		Crippen Method
mcvol	204.820	ml/mol	McGowan Method
rinpola	1856.00		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=R322955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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