

1-Phenyl-2-acetyl-4,4-dimethyl-3-pyrazolidone

Other names:	2-acetyl-4,4-dimethyl-1-phenylpyrazolidin-3-one
Inchi:	InChI=1S/C13H16N2O2/c1-10(16)15-12(17)13(2,3)9-14(15)11-7-5-4-6-8-11/h4-8H,9H2,1
InchiKey:	XWKAZXKJYHZGAI-UHFFFAOYSA-N
Formula:	C13H16N2O2
SMILES:	CC(=O)N1C(=O)C(C)(C)CN1c1ccccc1
Mol. weight [g/mol]:	232.28
CAS:	86475-37-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.823		Crippen Method
mcvol	182.510	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86475378&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

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