

2,4-dihydro-2,4,5-trimethyl-3H-pyrazol-3-one

Inchi:	InChI=1S/C6H10N2O/c1-4-5(2)7-8(3)6(4)9/h7H,1-3H3
InchiKey:	ZZQIPPXPEIMART-UHFFFAOYSA-N
Formula:	C6H10N2O
SMILES:	Cc1[nH]n(C)c(=O)c1C
Mol. weight [g/mol]:	126.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.35		Crippen Method
logp	-0.152		Crippen Method
mcvol	101.770	ml/mol	McGowan Method
ripol	1896.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R494892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices

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