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/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
ripol: Polar retention indices