

2-Pyrazoline, 1,3,5-trimethyl

Inchi: InChI=1S/C6H12N2/c1-5-4-6(2)8(3)7-5/h6H,4H2,1-3H3
InchiKey: RLPGNQZLVNPBIQ-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CC1=NN(C)C(C)C1
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.07		Crippen Method
logp	1.086		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
rinpol	832.00		NIST Webbook
rinpol	832.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R511081&Units=SI>

Legend

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

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