2-Pyrazoline, 1-ethyl-5-methyl

Inchi: InChI=1S/C6H12N2/c1-3-8-6(2)4-5-7-8/h5-6H,3-4H2,1-2H3
InchiKey: JSOODOAWWSZHPL-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CCN1N=CCC1C
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	845.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R511130&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