

n-Butylpyrazole

Inchi: InChI=1S/C7H12N2/c1-2-3-6-9-7-4-5-8-9/h4-5,7H,2-3,6H2,1H3
InchiKey: FMPJPCHSXGNEMD-UHFFFAOYSA-N
Formula: C7H12N2
SMILES: CCCCN1CCCN1
Mol. weight [g/mol]: 124.18
CAS: 52096-24-9

Physical Properties

Property code	Value	Unit	Source
affp	928.80	kJ/mol	NIST Webbook
basg	897.30	kJ/mol	NIST Webbook
log10ws	-2.34		Crippen Method
logp	1.683		Crippen Method
mcvol	109.990	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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=C52096249&Units=SI>

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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