4-NH2-pyrazole

Inchi: InChI=1S/C3H5N3/c4-3-1-5-6-2-3/h1-2H,4H2,(H,5,6)
InchiKey: AXINVSXSGNSVLV-UHFFFAOYSA-N
Formula: C3H5N3
SMILES: Nc1cn[nH]c1
Mol. weight [g/mol]: 83.09
CAS: 28466-26-4

Physical Properties

Property code	Value	Unit	Source
affp	907.60	kJ/mol	NIST Webbook
basg	874.00	kJ/mol	NIST Webbook
log10ws	-0.09		Crippen Method
logp	-0.490		Crippen Method
mcvol	63.610	ml/mol	McGowan Method

Sources

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=C28466264&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from: