1-azabicyclo[2.2.2]-octane, 3-cyano

Inchi: InChI=1S/C8H12N2/c9-5-8-6-10-3-1-7(8)2-4-10/h7-8H,1-4,6H2
InchiKey: ICSMHHPNBLZOLB-UHFFFAOYSA-N
Formula: C8H12N2
SMILES: N#CC1CN2CCC1CC2
Mol. weight [g/mol]: 136.19
CAS: 51627-76-0

Physical Properties

Property code	Value	Unit	Source
affp	935.40	kJ/mol	NIST Webbook
basg	904.60	kJ/mol	NIST Webbook
log10ws	-0.91		Crippen Method
logp	0.852		Crippen Method
mcvol	113.220	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=C51627760&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

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