

3-AMINOQUINUCLIDINE

Other names:	(+)-3-Aminoquinuclidine
Inchi:	InChI=1S/C7H14N2/c8-7-5-9-3-1-6(7)2-4-9/h6-7H,1-5,8H2
InchiKey:	REUAXQZIRFXQML-UHFFFAOYSA-N
Formula:	C7H14N2
SMILES:	NC1CN2CCC1CC2
Mol. weight [g/mol]:	126.20

Physical Properties

Property code	Value	Unit	Source
affp	985.50	kJ/mol	NIST Webbook
basg	954.70	kJ/mol	NIST Webbook
ie	7.96	eV	NIST Webbook
logp	0.039		Crippen Method
mcvol	107.730	ml/mol	McGowan Method
tb	459.60	K	Cheméo Relay (1.0)
tf	396.67	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6238148&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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