

Quinuclidine

Other names:	1-Azabicyclo[2.2.2]octane 1,4-Ethylenepiperidine 4-Azabicyclo[2.2.2]octane
Inchi:	InChI=1S/C7H13N/c1-4-8-5-2-7(1)3-6-8/h7H,1-6H2
InchiKey:	SBYHFKPVCBCYGV-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	C1CN2CCC1CC2
Mol. weight [g/mol]:	111.18
CAS:	100-76-5

Physical Properties

Property code	Value	Unit	Source
affp	983.30	kJ/mol	NIST Webbook
basg	952.50	kJ/mol	NIST Webbook
chs	-4557.42 ± 0.92	kJ/mol	NIST Webbook
hf	-4.30 ± 1.30	kJ/mol	NIST Webbook
hfs	-55.10 ± 1.20	kJ/mol	NIST Webbook
hsub	50.80	kJ/mol	NIST Webbook
hsub	50.80 ± 0.20	kJ/mol	NIST Webbook
ie	7.50	eV	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.50 ± 0.09	eV	NIST Webbook
ie	8.06 ± 0.01	eV	NIST Webbook
ie	8.02	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	1.102		Crippen Method
mcvol	97.750	ml/mol	McGowan Method
ss	206.98	J/molxK	NIST Webbook
tt	430.00 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cps	169.37	J/mol×K	298.15	NIST Webbook
hfust	5.86	kJ/mol	430.00	NIST Webbook
hfust	5.23	kJ/mol	196.00	NIST Webbook
hfust	5.86	kJ/mol	430.00	NIST Webbook
sfust	26.53	J/mol×K	196.00	NIST Webbook
sfust	13.81	J/mol×K	430.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100765&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tt:	Triple Point Temperature

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