3-Azabicyclo[3.2.2]nonane

Inchi: InChI=1S/C8H15N/c1-2-8-4-3-7(1)5-9-6-8/h7-9H,1-6H2
InchiKey: LICHZOBEUWVYSY-UHFFFAOYSA-N
Formula: C8H15N
SMILES: C1CC2CCC1CNC2
Mol. weight [g/mol]: 125.21
CAS: 283-24-9

Physical Properties

Property code	Value	Unit	Source
chs	-5190.29 ± 0.67	kJ/mol	NIST Webbook
gf	189.39	kJ/mol	Joback Method
hf	-43.68 ± 0.79	kJ/mol	NIST Webbook
hfs	-101.60 ± 0.67	kJ/mol	NIST Webbook
hfus	16.04	kJ/mol	Joback Method
hsub	57.90	kJ/mol	NIST Webbook
hsub	57.80 ± 1.30	kJ/mol	NIST Webbook
hvap	40.50	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.396		Crippen Method
mcvol	111.840	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
ss	245.73	J/mol×K	NIST Webbook
tb	457.28	K	Joback Method
tc	684.03	K	Joback Method
tf	310.27	K	Joback Method
tt	467.12 ± 0.01	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.04	J/mol×K	608.45	Joback Method
cpg	328.94	J/mol×K	646.24	Joback Method
cpg	243.63	J/mol×K	457.28	Joback Method

cpg	262.96	J/mol×K	495.07	Joback Method
cpg	281.10	J/mol×K	532.86	Joback Method
cpg	298.11	J/mol×K	570.66	Joback Method
cpg	342.87	J/mol×K	684.03	Joback Method
cps	237.80	J/mol×K	350.00	NIST Webbook
cps	239.03	J/mol×K	310.00	NIST Webbook
hfust	14.55	kJ/mol	297.80	NIST Webbook
hfust	6.92	kJ/mol	466.60	NIST Webbook
hfust	6.92	kJ/mol	466.60	NIST Webbook
hvapt	52.20	kJ/mol	373.00	NIST Webbook
sfust	14.82	J/mol×K	466.60	NIST Webbook
sfust	48.87	J/mol×K	297.80	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C283249&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure

sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume