8-Azabicyclo[3.2.1]oct-2-ene

Inchi: InChI=1S/C7H11N/c1-2-6-4-5-7(3-1)8-6/h1-2,6-8H,3-5H2
InchiKey: SURHOQQBDZIWSO-UHFFFAOYSA-N
Formula: C7H11N
SMILES: C1=CC2CCC(C1)N2
Mol. weight [g/mol]: 109.17
CAS: 5632-85-9

Physical Properties

Property code	Value	Unit	Source
gf	223.03	kJ/mol	Joback Method
hf	41.06	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	38.40	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.067		Crippen Method
mcvol	93.450	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
tb	436.50 ± 3.50	K	NIST Webbook
tc	652.57	K	Joback Method
tf	303.28	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.21	J/mol×K	429.29	Joback Method
cpg	203.07	J/mol×K	466.50	Joback Method
cpg	217.89	J/mol×K	503.72	Joback Method
cpg	231.72	J/mol×K	540.93	Joback Method
cpg	244.63	J/mol×K	578.14	Joback Method
cpg	256.66	J/mol×K	615.36	Joback Method
cpg	267.87	J/mol×K	652.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5632859&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume