2,3-Diazabicyclo[2.2.1]-hept-2-ene

Inchi: InChI=1S/C5H8N2/c1-2-5-3-4(1)6-7-5/h4-5H,1-3H2
InchiKey: IJDUBDHNOXAHCQ-UHFFFAOYSA-N
Formula: C5H8N2
SMILES: C1CC2CC1N=N2
Mol. weight [g/mol]: 96.13
CAS: 2721-32-6

Physical Properties

Property code	Value	Unit	Source
chs	-3262.90 ± 0.71	kJ/mol	NIST Webbook
gf	364.14	kJ/mol	Joback Method
hf	196.00	kJ/mol	NIST Webbook
hfs	152.10	kJ/mol	NIST Webbook
hfus	14.37	kJ/mol	Joback Method
hsub	43.90	kJ/mol	NIST Webbook
hsub	43.89	kJ/mol	NIST Webbook
hsub	55.30 ± 0.60	kJ/mol	NIST Webbook
hvap	39.43	kJ/mol	Joback Method
ie	8.94	eV	NIST Webbook
ie	8.45 ± 0.04	eV	NIST Webbook
ie	8.82	eV	NIST Webbook
log10ws	-1.19		Crippen Method
logp	1.373		Crippen Method
mcvol	75.250	ml/mol	McGowan Method
pc	5289.26	kPa	Joback Method
tb	438.11	K	Joback Method
tc	676.30	K	Joback Method
tf	322.31	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.35	J/mol×K	438.11	Joback Method

cpg	189.45	J/mol×K	477.81	Joback Method
cpg	204.50	J/mol×K	517.51	Joback Method
cpg	218.52	J/mol×K	557.21	Joback Method
cpg	231.55	J/mol×K	596.90	Joback Method
cpg	243.63	J/mol×K	636.60	Joback Method
cpg	254.80	J/mol×K	676.30	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=C2721326&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.