

Diaziridine, 3-ethyl-3-methyl-

Other names:	3-Ethyl-3-methyldiaziridine 3-Methyl-3-ethyldiaziridine c-C(CH ₃)(C ₂ H ₅)NHNH
Inchi:	InChI=1S/C4H10N2/c1-3-4(2)5-6-4/h5-6H,3H2,1-2H3
InchiKey:	MLTKZVHOZAKJMV-UHFFFAOYSA-N
Formula:	C ₄ H ₁₀ N ₂
SMILES:	CCC1(C)NN1
Mol. weight [g/mol]:	86.14
CAS:	4901-75-1

Physical Properties

Property code	Value	Unit	Source
affp	903.80	kJ/mol	NIST Webbook
basg	871.30	kJ/mol	NIST Webbook
gf	213.48	kJ/mol	Joback Method
hf	37.77	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	36.78	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	0.220		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	5273.90	kPa	Joback Method
tb	395.00	K	Joback Method
tc	605.25	K	Joback Method
tf	386.74	K	Joback Method
vc	0.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.69	J/mol×K	395.00	Joback Method
cpg	153.44	J/mol×K	430.04	Joback Method
cpg	163.33	J/mol×K	465.08	Joback Method
cpg	172.45	J/mol×K	500.13	Joback Method

cpg	180.90	J/mol×K	535.17	Joback Method
cpg	188.78	J/mol×K	570.21	Joback Method
cpg	196.17	J/mol×K	605.25	Joback Method

Sources

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=C4901751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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