

Diazirine, 3,3-diethyl

Inchi:	InChI=1S/C5H10N2/c1-3-5(4-2)6-7-5/h3-4H2,1-2H3
InchiKey:	AHUQTNIRSNOBTA-UHFFFAOYSA-N
Formula:	C5H10N2
SMILES:	CCC1(CC)N=N1
Mol. weight [g/mol]:	98.15

Physical Properties

Property code	Value	Unit	Source
gf	310.00	kJ/mol	Joback Method
hf	141.23	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	38.20	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.969		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
rmpol	653.00		NIST Webbook
tb	427.34	K	Joback Method
tc	646.95	K	Joback Method
tf	331.79	K	Joback Method
vc	0.354	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.85	J/mol×K	427.34	Joback Method
cpg	204.81	J/mol×K	463.94	Joback Method
cpg	217.74	J/mol×K	500.54	Joback Method
cpg	229.75	J/mol×K	537.15	Joback Method
cpg	240.93	J/mol×K	573.75	Joback Method
cpg	251.37	J/mol×K	610.35	Joback Method
cpg	261.18	J/mol×K	646.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R511452&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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