2,3-Pentamethylenediazirine

Inchi: InChI=1S/C6H10N2/c1-2-4-6(5-3-1)7-8-6/h1-5H2
InchiKey: ADJNKJMAEAJADP-UHFFFAOYSA-N
Formula: C6H10N2
SMILES: C1CCC2(CC1)N=N2
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
gf	362.68	kJ/mol	Joback Method
hf	201.41	kJ/mol	Joback Method
hfus	7.50	kJ/mol	Joback Method
hvap	40.99	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.113		Crippen Method
mcvol	89.340	ml/mol	McGowan Method
pc	5343.52	kPa	Joback Method
rinpol	756.00		NIST Webbook
tb	470.17	K	Joback Method
tc	725.98	K	Joback Method
tf	358.20	K	Joback Method
vc	0.352	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.61	J/mol×K	470.17	Joback Method
cpg	232.71	J/mol×K	512.80	Joback Method
cpg	249.18	J/mol×K	555.44	Joback Method
cpg	264.21	J/mol×K	598.07	Joback Method
cpg	277.98	J/mol×K	640.71	Joback Method
cpg	290.70	J/mol×K	683.34	Joback Method
cpg	302.54	J/mol×K	725.98	Joback Method

Sources

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=R120120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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