3,3-Dimethyldiazirine

Inchi: InChI=1S/C3H6N2/c1-3(2)4-5-3/h1-2H3
InchiKey: JYSCQQRNTHDPBR-UHFFFAOYSA-N
Formula: C3H6N2
SMILES: CC1(C)N=N1
Mol. weight [g/mol]: 70.09
CAS: 5161-49-9

Physical Properties

Property code	Value	Unit	Source
gf	293.16	kJ/mol	Joback Method
hf	182.51	kJ/mol	Joback Method
hfus	6.86	kJ/mol	Joback Method
hvap	33.75	kJ/mol	Joback Method
ie	9.76	eV	NIST Webbook
log10ws	-0.84		Crippen Method
logp	1.188		Crippen Method
mcvol	57.930	ml/mol	McGowan Method
pc	5981.40	kPa	Joback Method
rinpol	459.00		NIST Webbook
rinpol	459.00		NIST Webbook
tb	381.58	K	Joback Method
tc	606.42	K	Joback Method
tf	309.25	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	115.66	J/mol×K	381.58	Joback Method
cpg	127.09	J/mol×K	419.05	Joback Method
cpg	137.56	J/mol×K	456.53	Joback Method
cpg	147.14	J/mol×K	494.00	Joback Method
cpg	155.94	J/mol×K	531.48	Joback Method
cpg	164.06	J/mol×K	568.95	Joback Method

cpg	171.59	J/mol×K	606.42	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=C5161499&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
ie:	Ionization energy
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