2-Propyn-1-amine, N,N-dimethyl-

Other names:	N,N-Dimethyl-2-propyn-1-amine
	(CH3)2NCH2C«equiv»CH
	1-Dimethylamino-2-propyne
	3-Dimethylamino-1-propyne
	N,N-dimethyl propargylamine
	N-(2-Propynyl)-N,N-dimethylamine
	dimethyl(prop-2-ynyl)amine
Inchi:	InChI=1S/C5H9N/c1-4-5-6(2)3/h1H,5H2,2-3H3
InchiKey:	ILBIXZPOMJFOJP-UHFFFAOYSA-N
Formula:	C5H9N
SMILES:	C#CCN(C)C
Mol. weight [g/mol]:	83.13
CAS:	7223-38-3

Physical Properties

Property code	Value	Unit	Source
affp	940.30	kJ/mol	NIST Webbook
basg	909.50	kJ/mol	NIST Webbook
chl	-3451.40 ± 1.70	kJ/mol	NIST Webbook
gf	325.07	kJ/mol	Joback Method
hf	212.90	kJ/mol	Joback Method
hfl	197.60 ± 1.70	kJ/mol	NIST Webbook
hfus	14.70	kJ/mol	Joback Method
hvap	28.62	kJ/mol	Joback Method
ie	8.29 ± 0.03	eV	NIST Webbook
ie	8.17	eV	NIST Webbook
ie	8.22 ± 0.05	eV	NIST Webbook
log10ws	-0.28		Crippen Method
logp	0.181		Crippen Method
mcvol	82.690	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	637.00		NIST Webbook
tb	355.00	K	NIST Webbook
tb	354.20	K	NIST Webbook
tb	353.50 ± 0.50	K	NIST Webbook
tc	490.04	K	Joback Method
tf	225.55	K	Joback Method

vc	0.295	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.00	J/mol×K	316.36	Joback Method
cpg	138.89	J/mol×K	345.31	Joback Method
cpg	147.36	J/mol×K	374.25	Joback Method
cpg	155.42	J/mol×K	403.20	Joback Method
cpg	163.11	J/mol×K	432.15	Joback Method
cpg	170.42	J/mol×K	461.10	Joback Method
cpg	177.37	J/mol×K	490.04	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=C7223383&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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