

2-Propyn-1-amine, N-2-propynyl-

Other names:	Di-2-propynylamine Dipropargylamine (HC«equiv»CCH2)2NH
Inchi:	InChI=1S/C6H7N/c1-3-5-7-6-4-2/h1-2,7H,5-6H2
InchiKey:	RGSODMOUXWISAG-UHFFFAOYSA-N
Formula:	C6H7N
SMILES:	C#CCNCC#C
Mol. weight [g/mol]:	93.13
CAS:	6921-28-4

Physical Properties

Property code	Value	Unit	Source
affp	910.00	kJ/mol	NIST Webbook
basg	876.90	kJ/mol	NIST Webbook
gf	535.17	kJ/mol	Joback Method
hf	470.10	kJ/mol	Joback Method
hfl	429.70 ± 4.20	kJ/mol	NIST Webbook
hfus	22.35	kJ/mol	Joback Method
hvap	35.10	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	-0.158		Crippen Method
mcvol	88.180	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	367.09	K	Joback Method
tc	562.91	K	Joback Method
tf	303.98	K	Joback Method
vc	0.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.54	J/mol×K	367.09	Joback Method
cpg	160.59	J/mol×K	399.73	Joback Method
cpg	168.18	J/mol×K	432.36	Joback Method

cpg	175.33	J/mol×K	465.00	Joback Method
cpg	182.08	J/mol×K	497.63	Joback Method
cpg	188.43	J/mol×K	530.27	Joback Method
cpg	194.42	J/mol×K	562.91	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	336.70	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6921284&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hfl:	Liquid phase 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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