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

Other names:	Tripropargylamine
	Tri-2-propynylamine
	(HC«equiv»CCH2)3N
	Tris(2-propynyl)amine
	tris(propyn-2-yl)amine
Inchi:	InChI=1S/C9H9N/c1-4-7-10(8-5-2)9-6-3/h1-3H,7-9H2
InchiKey:	ZHOBJWVNWMQMLF-UHFFFAOYSA-N
Formula:	C9H9N
SMILES:	C#CCN(CC#C)CC#C
Mol. weight [g/mol]:	131.17
CAS:	6921-29-5

Physical Properties

Property code	Value	Unit	Source
affp	925.20	kJ/mol	NIST Webbook
basg	894.40	kJ/mol	NIST Webbook
chl	-5642.12 ± 0.42	kJ/mol	NIST Webbook
gf	804.89	kJ/mol	Joback Method
hf	714.14	kJ/mol	Joback Method
hfl	814.20 ± 0.40	kJ/mol	NIST Webbook
hfl	671.10 ± 5.90	kJ/mol	NIST Webbook
hfus	31.01	kJ/mol	Joback Method
hvap	37.25	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.188		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	388.12	K	Joback Method
tc	587.22	K	Joback Method
tf	364.57	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.15	J/mol×K	388.12	Joback Method
cpg	234.28	J/mol×K	421.30	Joback Method
cpg	244.69	J/mol×K	454.49	Joback Method
cpg	254.42	J/mol×K	487.67	Joback Method
cpg	263.50	J/mol×K	520.86	Joback Method
cpg	271.99	J/mol×K	554.04	Joback Method
cpg	279.92	J/mol×K	587.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.20	K	1.50	NIST Webbook

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=C6921295&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
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