2-Propyn-1-amine, N,N-diethyl-

Other names:	2-Propynylamine, N,N-diethyl-
	Diethylpropargylamine
	N,N-Diethyl-2-propynylamine
	N,N-Diethylpropargylamine
	1-N,N-Diethylamino-2-propyne
	3-(Diethylamino)propyne
	3-(N,N-Diethylamino)propyne
	1-Diethylaminopropyne-2
	3-Diethylamino-1-propyne
	1-Diethylamino-2-propyne
	NSC 63868
Inchi:	InChI=1S/C7H13N/c1-4-7-8(5-2)6-3/h1H,5-7H2,2-3H3
InchiKey:	JZJXKEWVUBVOEH-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	C#CCN(CC)CC
Mol. weight [g/mol]:	111.18
CAS:	4079-68-9

Physical Properties

Property code	Value	Unit	Source
gf	341.91	kJ/mol	Joback Method
hf	171.62	kJ/mol	Joback Method
hfus	19.88	kJ/mol	Joback Method
hvap	33.08	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.961		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	757.00		NIST Webbook
rinpol	757.00		NIST Webbook
tb	362.12	K	Joback Method
tc	536.13	K	Joback Method
tf	248.09	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.70	J/mol×K	362.12	Joback Method
cpg	209.38	J/mol×K	391.12	Joback Method
cpg	220.53	J/mol×K	420.12	Joback Method
cpg	231.16	J/mol×K	449.13	Joback Method
cpg	241.30	J/mol×K	478.13	Joback Method
cpg	250.97	J/mol×K	507.13	Joback Method
cpg	260.18	J/mol×K	536.13	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=C4079689&Units=SI

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