2-Propen-1-amine, N-2-propenyl-

Other names:	Diallylamine
	Di-2-propenylamine
	(CH2=CHCH2)2NH
	UN 2359
	N,N-Di(2-propenyl)amine
Inchi:	InChI=1S/C6H11N/c1-3-5-7-6-4-2/h3-4,7H,1-2,5-6H2
InchiKey:	DYUWTXWIYMHBQS-UHFFFAOYSA-N
Formula:	C6H11N
SMILES:	C=CCNCC=C
Mol. weight [g/mol]:	97.16
CAS:	124-02-7

Physical Properties

Property code	Value	Unit	Source
affp	949.30	kJ/mol	NIST Webbook
basg	916.30	kJ/mol	NIST Webbook
gf	264.71	kJ/mol	Joback Method
hf	137.16	kJ/mol	Joback Method
hfus	13.83	kJ/mol	Joback Method
hvap	34.05	kJ/mol	Joback Method
ie	8.80 ± 0.30	eV	NIST Webbook
ie	8.79	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	0.948		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	660.00		NIST Webbook
tb	384.20	K	NIST Webbook
tc	557.28	K	Joback Method
tf	206.52	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.58	J/mol×K	380.21	Joback Method
cpg	180.78	J/mol×K	409.72	Joback Method
cpg	190.52	J/mol×K	439.23	Joback Method
cpg	199.81	J/mol×K	468.74	Joback Method
cpg	208.67	J/mol×K	498.25	Joback Method
cpg	217.11	J/mol×K	527.77	Joback Method
cpg	225.15	J/mol×K	557.28	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C124027&Units=SI
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

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
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

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