

2-Propen-1-amine, 2-methyl-

Other names:	2-methylprop-2-en-1-ylamine CH ₂ =C(CH ₃)CH ₂ NH ₂ Methallylamine
Inchi:	InChI=1S/C4H9N/c1-4(2)3-5/h1,3,5H2,2H3
InchiKey:	VXDHQYLFEYUMFY-UHFFFAOYSA-N
Formula:	C ₄ H ₉ N
SMILES:	C=C(C)CN
Mol. weight [g/mol]:	71.12
CAS:	2878-14-0

Physical Properties

Property code	Value	Unit	Source
affp	917.50	kJ/mol	NIST Webbook
basg	883.50	kJ/mol	NIST Webbook
gf	128.54	kJ/mol	Joback Method
hf	23.54	kJ/mol	Joback Method
hfus	8.72	kJ/mol	Joback Method
hvap	34.55	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-0.78		Crippen Method
logp	0.521		Crippen Method
mcvol	72.900	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	360.01	K	Joback Method
tc	549.60	K	Joback Method
tf	202.38	K	Joback Method
vc	0.271	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.39	J/mol×K	360.01	Joback Method
cpg	133.50	J/mol×K	391.61	Joback Method
cpg	141.24	J/mol×K	423.21	Joback Method

cpg	148.62	J/mol×K	454.80	Joback Method
cpg	155.67	J/mol×K	486.40	Joback Method
cpg	162.38	J/mol×K	518.00	Joback Method
cpg	168.78	J/mol×K	549.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2878140&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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1405.mol

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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