

1,1-Dimethylamino-1-butene

Other names:	(CH3)2NCH=CHC2H5
Inchi:	InChI=1S/C6H13N/c1-4-5-6-7(2)3/h5-6H,4H2,1-3H3/b6-5+
InchiKey:	XWAKKPDDQPWGAQ-AATRIKPKSA-N
Formula:	C6H13N
SMILES:	CCC=CN(C)C
Mol. weight [g/mol]:	99.17
CAS:	14548-12-0

Physical Properties

Property code	Value	Unit	Source
gf	190.64	kJ/mol	Joback Method
hf	17.58	kJ/mol	Joback Method
hfus	14.52	kJ/mol	Joback Method
hvap	30.95	kJ/mol	Joback Method
ie	7.57	eV	NIST Webbook
log10ws	-1.25		Crippen Method
logp	1.472		Crippen Method
mcvol	101.080	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
tb	353.28	K	Joback Method
tc	524.57	K	Joback Method
tf	184.77	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.25	J/mol×K	353.28	Joback Method
cpg	181.94	J/mol×K	381.83	Joback Method
cpg	193.10	J/mol×K	410.38	Joback Method
cpg	203.73	J/mol×K	438.92	Joback Method
cpg	213.86	J/mol×K	467.47	Joback Method
cpg	223.51	J/mol×K	496.02	Joback Method
cpg	232.69	J/mol×K	524.57	Joback Method

Sources

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=C14548120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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