

2-Propen-1-amine, N-ethyl-N-methyl-

Other names:	2-Propeneamine, N-ethyl-N-methyl
Inchi:	InChI=1S/C6H13N/c1-4-6-7(3)5-2/h4H,1,5-6H2,2-3H3
InchiKey:	LQVWXFHNYICENT-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	C=CCN(C)CC
Mol. weight [g/mol]:	99.17
CAS:	107995-54-0

Physical Properties

Property code	Value	Unit	Source
gf	198.26	kJ/mol	Joback Method
hf	25.79	kJ/mol	Joback Method
hfus	13.04	kJ/mol	Joback Method
hvap	30.32	kJ/mol	Joback Method
log10ws	-0.76		Crippen Method
logp	1.124		Crippen Method
mcvol	101.080	ml/mol	McGowan Method
pc	3250.43	kPa	Joback Method
rinpol	668.00		NIST Webbook
rinpol	668.00		NIST Webbook
tb	345.80	K	Joback Method
tc	511.63	K	Joback Method
tf	188.09	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.48	J/mol×K	345.80	Joback Method
cpg	181.74	J/mol×K	373.44	Joback Method
cpg	192.52	J/mol×K	401.08	Joback Method
cpg	202.85	J/mol×K	428.71	Joback Method
cpg	212.73	J/mol×K	456.35	Joback Method
cpg	222.19	J/mol×K	483.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C107995540&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

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