

Butanamine, 2-methyl-N-ethylidene

Other names:	1-Butanamine, 2-methyl-N-ethylidene
Inchi:	InChI=1S/C7H15N/c1-4-7(3)6-8-5-2/h5,7H,4,6H2,1-3H3
InchiKey:	QVGCELKIEZJTAN-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CC=NCC(C)CC
Mol. weight [g/mol]:	113.20

Physical Properties

Property code	Value	Unit	Source
hf	-110.87	kJ/mol	Joback Method
hvap	34.10	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	2.123		Crippen Method
mcvol	115.170	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	787.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	790.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	957.00		NIST Webbook
tb	435.80	K	Joback Method
tc	626.17	K	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=R45724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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