

Ethanamine, N-butylidene-

Other names:	Ethylamine, N-butylidene- n-C3H7CH=NC2H5
Inchi:	InChI=1S/C6H13N/c1-3-5-6-7-4-2/h6H,3-5H2,1-2H3
InchiKey:	BLARBXSPVIJGSG-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	CCCC=NCC
Mol. weight [g/mol]:	99.17
CAS:	1611-12-7

Physical Properties

Property code	Value	Unit	Source
affp	955.50	kJ/mol	NIST Webbook
basg	923.00	kJ/mol	NIST Webbook
hf	-84.95	kJ/mol	Joback Method
hvap	32.26	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.877		Crippen Method
mvol	101.080	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	413.36	K	Joback Method
tc	601.00	K	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1611127&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
hf:	Enthalpy of formation 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

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