

Butanamide, 3-methyl-N-(2-methylpropylidene)

Other names:	N-(2-Methylpropylidene)-butylamine
Inchi:	InChI=1S/C8H17N/c1-4-5-6-9-7-8(2)3/h7-8H,4-6H2,1-3H3
InchiKey:	ICXVVVQXAMOEJE-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCCCN=CC(C)C
Mol. weight [g/mol]:	127.23
CAS:	6898-75-5

Physical Properties

Property code	Value	Unit	Source
chl	-5417.00 ± 10.00	kJ/mol	NIST Webbook
chl	-5444.80 ± 3.40	kJ/mol	NIST Webbook
hf	-91.20 ± 5.40	kJ/mol	NIST Webbook
hfl	-133.00 ± 3.00	kJ/mol	NIST Webbook
hvap	42.00 ± 2.00	kJ/mol	NIST Webbook
hvap	41.80	kJ/mol	NIST Webbook
log10ws	-2.09		Crippen Method
logp	2.513		Crippen Method
mcvol	129.260	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	926.00		NIST Webbook
rinpol	927.00		NIST Webbook
tb	458.68	K	Joback Method
tc	647.16	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	42.00 ± 2.00	kJ/mol	293.00	NIST Webbook

Sources

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=C6898755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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

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