

1-Butanol, 4-amino, N-isopropylidene

Inchi:	InChI=1S/C7H15NO/c1-7(2)8-5-3-4-6-9/h9H,3-6H2,1-2H3
InchiKey:	OXCGFXIXXWMYDA-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CC(C)=NCCCCO
Mol. weight [g/mol]:	129.20

Physical Properties

Property code	Value	Unit	Source
hf	-267.61	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.240		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinpol	1115.00		NIST Webbook
tb	528.30	K	Joback Method
tc	708.84	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=R64738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

hf:	Enthalpy of formation 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

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