

2-Propanone - propanal azine

Inchi: InChI=1S/C6H12N2/c1-4-5-7-8-6(2)3/h5H,4H2,1-3H3/b7-5+
InchiKey: QLPCIZRSHRVZSJ-FNORWQNLSA-N
Formula: C6H12N2
SMILES: CCC=NN=C(C)C
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
hf	-12.52	kJ/mol	Joback Method
hvap	35.66	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.863		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	828.00		NIST Webbook
tb	489.92	K	Joback Method
tc	702.60	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=R511061&Units=SI>

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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