

Propanal, isopropyl hydrazone, # 1

Inchi: InChI=1S/C6H14N2/c1-4-5-7-8-6(2)3/h5-6,8H,4H2,1-3H3/b7-5+
InchiKey: XWSLKTSKRPZHPI-FNORWQNLSA-N
Formula: C6H14N2
SMILES: CCC=NNC(C)C
Mol. weight [g/mol]: 114.19

Physical Properties

Property code	Value	Unit	Source
hf	-36.76	kJ/mol	Joback Method
hvap	38.31	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	1.380		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpole	838.00		NIST Webbook
rinpole	838.00		NIST Webbook
tb	463.09	K	Joback Method
tc	658.51	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=R512039&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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