

2-Propanone, methylhydrazone

Other names:	Acetone methylhydrazone
Inchi:	InChI=1S/C4H10N2/c1-4(2)6-5-3/h5H,1-3H3
InchiKey:	JXSSEZYJBTUIGX-UHFFFAOYSA-N
Formula:	C4H10N2
SMILES:	CNN=C(C)C
Mol. weight [g/mol]:	86.14
CAS:	5771-02-8

Physical Properties

Property code	Value	Unit	Source
chl	-3043.90 ± 0.80	kJ/mol	NIST Webbook
hf	0.01	kJ/mol	Joback Method
hfl	39.70 ± 0.80	kJ/mol	NIST Webbook
hvap	34.33	kJ/mol	Joback Method
ie	7.69	eV	NIST Webbook
log10ws	-0.84		Crippen Method
logp	0.602		Crippen Method
mcvol	82.880	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	728.00		NIST Webbook
rinpol	728.00		NIST Webbook
tb	417.65	K	Joback Method
tc	616.64	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=C5771028&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
ie:	Ionization energy
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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<https://www.chemeo.com/cid/27-829-2/2-Propanone-methylhydrazone.pdf>

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