

Acetic acid isopropylidene-hydrazone

Other names:	Acetone, acetylhydrazone
Inchi:	InChI=1S/C5H10N2O/c1-4(2)6-7-5(3)8/h1-3H3,(H,7,8)
InchiKey:	XLHDGJPPMZUJIM-UHFFFAOYSA-N
Formula:	C5H10N2O
SMILES:	CC(=O)NN=C(C)C
Mol. weight [g/mol]:	114.15
CAS:	3742-63-0

Physical Properties

Property code	Value	Unit	Source
hf	-133.21	kJ/mol	Joback Method
hvap	43.30	kJ/mol	Joback Method
log10ws	-1.03		Crippen Method
logp	0.518		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1267.00		NIST Webbook
tb	494.40	K	Joback Method
tc	702.03	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=C3742630&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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