

Acetamide, N-methyl-N-nitroso-

Inchi: InChI=1S/C3H6N2O2/c1-3(6)5(2)4-7/h1-2H3
InchiKey: FFLFWNRFMZRFKU-UHFFFAOYSA-N
Formula: C3H6N2O2
SMILES: CC(=O)N(C)N=O
Mol. weight [g/mol]: 102.09
CAS: 7417-67-6

Physical Properties

Property code	Value	Unit	Source
hf	-318.49	kJ/mol	Joback Method
hvap	40.16	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	0.146		Crippen Method
mcvol	76.230	ml/mol	McGowan Method
pc	4672.09	kPa	Joback Method
rinpol	684.00		NIST Webbook
rinpol	684.00		NIST Webbook
tb	397.75	K	Joback Method
tc	578.55	K	Joback Method

Sources

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=C7417676&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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