

2-Propanamine, N-methyl-N-nitroso-

Other names:	Ethylamine, N,1-dimethyl-N-nitroso- Isopropylmethylnitrosamine Methylisopropylnitrosamine N-Methyl-N-nitrosoisopropylamine N,1-Dimethyl-N-nitrosoethanamine
Inchi:	InChI=1S/C4H10N2O/c1-4(2)6(3)5-7/h4H,1-3H3
InchiKey:	KQDYNYCCEGQPTN-UHFFFAOYSA-N
Formula:	C4H10N2O
SMILES:	CC(C)N(C)N=O
Mol. weight [g/mol]:	102.14
CAS:	30533-08-5

Physical Properties

Property code	Value	Unit	Source
hf	-231.83	kJ/mol	Joback Method
hvap	35.25	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.008		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinsol	855.00		NIST Webbook
tb	366.32	K	Joback Method
tc	537.09	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=C30533085&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
r_{inpol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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