

2-Propanamine, N-(1-methylethyl)-N-nitroso-

Other names:	Diethylamine, 1,1'-dimethyl-N-nitroso- Diisopropylnitrosamine N-Nitrosodiisopropylamine Diisopropylamine, N-nitroso- Diisopropylnitrosamin Nitrosodiisopropylamine
Inchi:	InChI=1S/C6H14N2O/c1-5(2)8(7-9)6(3)4/h5-6H,1-4H3
InchiKey:	AUIKJTGFPLMFP-UHFFFAOYSA-N
Formula:	C6H14N2O
SMILES:	CC(C)N(N=O)C(C)C
Mol. weight [g/mol]:	130.19
CAS:	601-77-4

Physical Properties

Property code	Value	Unit	Source
hf	-278.39	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
ie	8.58	eV	NIST Webbook
log10ws	-2.31		Crippen Method
logp	1.787		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpola	979.00		NIST Webbook
tb	411.64	K	Joback Method
tc	585.13	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=C601774&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ie:	Ionization energy
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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