

Urea, N-methyl-N-nitroso-

Other names:	1-Methyl-1-Nitrosourea
	1-Methyl-1-nitrosomocovina
	1-nitroso-1-methylurea
	Carbamide, N-methyl-N-nitroso-
	MNU
	Methylnitroso-harnstoff
	Methylnitrosourea
	Methylnitrosouree
	N-Methyl-N-nitroso-harnstoff
	N-Methyl-N-nitrosourea
	N-Nitroso-N-methyl-harnstoff
	N-Nitroso-N-methylcarbamide
	N-Nitroso-N-methylurea
	NMH
	NMU
	NSC 23909
	Nitrosomethylurea
	Rcra waste number U177
	SKI 24464
	SRI 859
	Urea, 1-methyl-1-nitroso-
Inchi:	InChI=1S/C2H5N3O2/c1-5(4-7)2(3)6/h1H3,(H2,3,6)
InchiKey:	ZRKWMRDKSOPRRS-UHFFFAOYSA-N
Formula:	C2H5N3O2
SMILES:	CN(N=O)C(N)=O
Mol. weight [g/mol]:	103.08
CAS:	684-93-5

Physical Properties

Property code	Value	Unit	Source
hf	-264.06	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-0.85		Aqueous Solubility Prediction Method
logp	-0.322		Crippen Method
mcvol	72.120	ml/mol	McGowan Method
pc	5827.17	kPa	Joback Method

tb	447.40	K	Joback Method
tc	644.00	K	Joback Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C684935&Units=SI>

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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