Urea, trimethylnitroso-

Other names: N-Nitrosotrimethylurea
                          N-Trimethylnitrosourea
                          Nitrosotrimethylurea
                          Trimethylnitrosourea
                          Urea, 1,1,3-trimethyl-3-nitroso-
                          N-Nitroso-trimethylharnstoff
                          Trimethylnitrosoharnstoff
                          Trimethylnitrosomocovina
                          N-Trimethyl-N-nitrosourea
                          1,1,3-Trimethyl-3-nitrosourea
                          Urea, N,N,N'-trimethyl-N'-nitroso-

Inchi: InChI=1S/C4H9N3O2/c1-6(2)4(8)7(3)5-9/h1-3H3
InchiKey: LOEHVDVYTQIWEV-UHFFFAOYSA-N
Formula: C4H9N3O2
SMILES: CN(C)C(=O)N(C)N=O
Mol. weight [g/mol]: 131.13
CAS: 3475-63-6

Physical Properties

Property code	Value	Unit	Source
hf	-271.60	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-0.57		Crippen Method
logp	0.281		Crippen Method
mcvol	100.300	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	433.07	K	Joback Method
tc	610.97	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3475636&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	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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