1,3-Dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinon

Other names:	1,3-Dimethyl-tetrahydro-2(1H)-pyrimidone 1,3-Dimethyltetrahydro-2(1H)-pyrimidinone 1,3-dimethylpropyleneurea 2(1H)-Pyrimidinone, tetrahydro-1,3-dimethyl- 2(1H)-pryminidone, 3,4,5,6-tetrahydro-1,3-dimethyl- N,N'-Dimethyltrimethyleneurea Tetrahydro-1,3-dimethyl-2(1H)pyrimidin-2-onee tetrahydro-1,3-dimethyl-1H-pyrimidin-2-one
Inchi:	InChI=1S/C6H12N2O/c1-7-4-3-5-8(2)6(7)9/h3-5H2,1-2H3
InchiKey:	GUVUOGQBMYCBQP-UHFFFAOYSA-N
Formula:	C6H12N2O
SMILES:	CN1CCCN(C)C1=O
Mol. weight [g/mol]:	128.17
CAS:	7226-23-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	0.374		Crippen Method
mcvol	106.070	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
rhol	1076.18	kg/m3	278.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K

rhol	1067.81	kg/m3	288.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K
rhol	1059.46	kg/m3	298.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K
rhol	1051.12	kg/m3	308.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K
rhol	1046.95	kg/m3	313.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K
rhol	1042.78	kg/m3	318.15	Volume-related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K
rhol	1065.00	kg/m3	293.15	Investigation of the Solubilities of Carbon Dioxide in Some Low Volatile Solvents and Their Thermodynamic Properties

Sources

Solubility and thermodynamic properties of SO2 in three low volatile solvents and their Thermodynamic Properties:	https://www.doi.org/10.1016/j.jct.2016.05.004
Volume related interaction parameters for dilute solutions of 1,3-dimethylpropyleneurea in normal and heavy water between 278.15 K and 318.15 K:	https://www.doi.org/10.1016/j.tca.2010.11.002
Enthalpy related interaction parameters in H2O isotopically distinguishable aqueous solutions of tetramethylurea cyclic derivatives at 298.15 K:	https://www.doi.org/10.1016/j.tca.2011.05.019
Investigation of the solubilities of Carbon Dioxide in Some Low Volatile Solvents and Their Thermodynamic Properties:	https://www.doi.org/10.1021/acs.jced.5b00893
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7226235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhol:	Liquid Density