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

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 H/D isotopically distinguishable aqueous solutions of tetramethylurea 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 Cyclic Urea Derivatives at 298.15 K:	https://www.doi.org/10.1021/acs.jced.5b00893
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Solvents and Their Thermodynamic Properties:	
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
Solubility and thermodynamic properties of SO2 in three low volatile urea derivatives:	https://www.doi.org/10.1016/j.jct.2016.05.004

Legend

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

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