

2H-Azepin-2-one, hexahydro-1-methyl-

Other names:	1-methylazacycloheptan-2-one 1-methylcaprolactam 1-methylhexahydro-2H-azepin-2-one 2H-Azepin-2-one, hexahydro-N-methyl- Hexahydro-1-methyl-2H-azepin-2-one N-Methyl-ε-caprolactam N-Methyl-«epsilon»-caprolactam N-methyl-epsilon.-caprolactam N-methylcaprolactam NSC 68794 «epsilon»-Caprolactam, N-methyl-
Inchi:	InChI=1S/C7H13NO/c1-8-6-4-2-3-5-7(8)9/h2-6H2,1H3
InchiKey:	ZWXPDGCFMMFNW-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CN1CCCCC1=O
Mol. weight [g/mol]:	127.18
CAS:	2556-73-2

Physical Properties

Property code	Value	Unit	Source
chl	-4305.80 ± 0.40	kJ/mol	NIST Webbook
chl	-4304.10	kJ/mol	NIST Webbook
ie	8.73	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-0.99		Crippen Method
logp	1.019		Crippen Method
mvol	110.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	49.40	kJ/mol	370.00	NIST Webbook

pvap	12.84	kPa	434.66	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	4.39	kPa	405.13	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	5.65	kPa	411.63	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	6.53	kPa	415.53	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	7.91	kPa	420.70	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	8.99	kPa	424.29	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	10.38	kPa	428.38	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	11.12	kPa	430.35	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	4.02	kPa	402.95	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	13.60	kPa	436.35	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane

pvap	16.89	kPa	443.09	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	21.39	kPa	450.68	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	26.82	kPa	458.30	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	30.50	kPa	462.79	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	36.27	kPa	468.95	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	47.69	kPa	479.21	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane
pvap	101.40	kPa	510.60	Vapor Pressures of 1-Methyl-2-pyrrolidone, 1-Methyl-azepan-2-one, and 1,2-Epoxy-3-chloropropane

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	0.80	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
High-Pressure Phase Behavior of CO₂ + N-Vinyl Caprolactam and CO₂ + N-Vinyl Caprolactam Systems: <https://www.doi.org/10.1021/je0495334>
High-Pressure Phase Behavior of 1-Methyl-2-pyrrolidone, N-Methylazepan-2-one, and 1,2-Epoxy-3-chloropropane: <https://www.doi.org/10.1021/je700398k>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2556732&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

chl: Standard liquid enthalpy of combustion
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure
tbrp: Boiling point at reduced pressure

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