

Pyrimido[1,2-a]azepine, 2,3,4,6,7,8,9,10-octahydro-

Other names:

1,5-Diaza(5,4,0)undec-5-ene
1,5-Diazabicyclo[5.4.0]-5-undecene
1,5-Diazabicyclo[5.4.0]undec-5-ene
1,8-Diazabicyclo[5.4.0]undec-7-ene
1,8-diaza-7-bicyclo[5.4.0]undecene
2,3,4,6,7,8,9,10-Octahydropyrimido(1,2-«alpha»)azepine
2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine

DBU

Diazabicycloundecene

Inchi: InChI=1S/C9H16N2/c1-2-5-9-10-6-4-8-11(9)7-3-1/h1-8H2

InchiKey: GQHTUMJGOHRCHB-UHFFFAOYSA-N

Formula: C9H16N2

SMILES: C1CCC2=NCCCN2CC1

Mol. weight [g/mol]: 152.24

CAS: 6674-22-2

Physical Properties

Property code	Value	Unit	Source
affp	1047.90	kJ/mol	NIST Webbook
basg	1015.50	kJ/mol	NIST Webbook
log10ws	-1.61		Crippen Method
logp	1.665		Crippen Method
mcvol	131.610	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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dvisc	0.0153500	Paxs	288.10	Studies on viscosity and conductivity of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 328.1 K
dvisc	0.0049100	Paxs	328.10	Studies on viscosity and conductivity of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 328.1 K
dvisc	0.0060800	Paxs	318.10	Studies on viscosity and conductivity of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 328.1 K
dvisc	0.0081700	Paxs	308.10	Studies on viscosity and conductivity of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 328.1 K
dvisc	0.0103200	Paxs	298.10	Studies on viscosity and conductivity of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 328.1 K

rhol	998.40	kg/m3	323.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1007.40	kg/m3	308.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1014.10	kg/m3	298.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1000.80	kg/m3	318.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	994.20	kg/m3	328.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1017.10	kg/m3	293.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K

rhol	1010.90	kg/m3	303.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1004.60	kg/m3	313.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K
rhol	1019.84	kg/m3	293.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1016.15	kg/m3	298.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1012.45	kg/m3	303.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1008.73	kg/m3	308.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1005.00	kg/m3	313.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	970.60	kg/m3	358.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	997.48	kg/m3	323.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions

rhol	993.69	kg/m3	328.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	989.89	kg/m3	333.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	986.06	kg/m3	338.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	982.22	kg/m3	343.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	978.37	kg/m3	348.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	974.49	kg/m3	353.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1001.25	kg/m3	318.15	Measurements and modeling of CO2 solubility in 1,8-diazabicyclo-[5.4.0]-undec-7-ene - glycerol solutions
rhol	1020.60	kg/m3	288.15	Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K

srf	0.04	N/m	323.10	Studies on surface tension of 1,8-diazabicyclo [5.4.0] undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 323.1 K
srf	0.04	N/m	318.10	Studies on surface tension of 1,8-diazabicyclo [5.4.0] undec-7-ene (DBU)-glycerol and CO2-DBU-glycerol solutions at temperatures from 288.1 K to 323.1 K
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	375.77	K	0.51	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling

tbp	383.45	K	0.71	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	389.40	K	1.01	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	395.15	K	1.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	397.75	K	1.51	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	400.85	K	1.71	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	403.95	K	2.01	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	407.05	K	2.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling

tbp	409.00	K	2.51	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	412.87	K	3.01	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	416.15	K	3.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	416.95	K	3.51	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	421.02	K	4.01	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	422.22	K	4.21	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	424.13	K	4.51	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling

tbp	426.92	K	5.01	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	427.85	K	5.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	432.45	K	6.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	437.20	K	7.31	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbrp	354.70	K	0.08	NIST Webbook

Sources

Density studies of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBN) and CO₂-DBU-glycerol solutions at temperatures between 288.15 K and 328.15 K:

<https://www.doi.org/10.1016/j.jct.2018.03.017>

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C6674222&Units=SI>

<https://www.doi.org/10.1016/j.jct.2018.05.013>

<https://www.doi.org/10.1016/j.jct.2019.04.017>

<https://www.doi.org/10.1016/j.fluid.2014.04.021>

https://www.chemeo.com/doc/models/crippen_log10ws

<https://www.doi.org/10.1016/j.fluid.2015.08.008>

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

Studies on surface tension of 1,8-diazabicyclo [5.4.0] undec-7-ene (DBN) and CO₂-DBU-glycerol solutions at temperatures from 288.1 K to 320.4 K:

Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN + water + DBU systems for cellulose solvent recycling:

Legend

affp:	Proton affinity
basg:	Gas basicity
dvisc:	Dynamic viscosity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rhol:	Liquid Density
srf:	Surface Tension
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure

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