1,5-Diazabicyclo[4.3.0]non-5-ene

Other names:	1,5-diazobicyclo[4.3.0]non-5-ene
	2,3,4,6,7,8-hexahydropyrrolo[1,2-a]pyrimidine
	Pyrrolo[1,2-a]pyrimidine, 2,3,4,6,7,8-hexahydro-
Inchi:	InChI=1S/C7H12N2/c1-3-7-8-4-2-6-9(7)5-1/h1-6H2
InchiKey:	SGUVLZREKBPKCE-UHFFFAOYSA-N
Formula:	C7H12N2
SMILES:	C1CN=C2CCCN2C1
Mol. weight [g/mol]:	124.18
CAS:	3001-72-7

Physical Properties

Property code	Value	Unit	Source
affp	1038.30	kJ/mol	NIST Webbook
basg	1005.90	kJ/mol	NIST Webbook
log10ws	-0.77		Crippen Method
logp	0.884		Crippen Method
mcvol	103.430	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	358.84	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	364.01	K	0.91	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling

tbp	364.61	K	0.92	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	371.35	K	1.39	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	372.05	K	1.41	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	379.14	K	1.87	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	387.20	K	2.81	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	387.81	K	2.86	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	
tbp	390.96	K	3.37	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling	

tbp	393.33	K	3.88	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	400.15	K	5.11	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	402.06	K	5.53	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	404.85	K	6.11	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	407.93	K	7.15	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	412.15	K	8.11	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	415.55	K	9.40	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling

tbp	417.65	K	10.12	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbp	422.75	K	12.14	Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling
tbrp	369.70	K	1.00	NIST Webbook

Sources

Dew points of pure DBN and DBU and vapor-liquid equilibria of water + DBN and water + DBU systems for cellulose solvent recycling:	https://www.doi.org/10.1016/j.fluid.2015.08.008
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3001727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure

Latest version available from:
https://www.chemeo.com/cid/53-454-9/1-5-Diazabicyclo-4-3-0-non-5-ene.pdf
Generated by Cheméo on 2025-12-05 18:08:19.598368905 +0000 UTC m=+4706297.128409560.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.