

1H-Imidazole, 1-propyl-

Other names:	1-propyl-1H-imidazole 1-propylimidazole N-propylimidazole
Inchi:	InChI=1S/C6H10N2/c1-2-4-8-5-3-7-6-8/h3,5-6H,2,4H2,1H3
InchiKey:	IYVYLVCVXXCYRI-UHFFFAOYSA-N
Formula:	C6H10N2
SMILES:	CCCN1CCN1
Mol. weight [g/mol]:	110.16
CAS:	35203-44-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	1.293		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
rmpol	1068.00		NIST Webbook
ripol	1768.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	2.59e-03	kPa	279.10	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	3.83e-03	kPa	283.40	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	5.89e-03	kPa	288.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

pvap	7.00e-03	kPa	290.40	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	8.81e-03	kPa	293.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.01	kPa	296.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.01	kPa	298.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.02	kPa	301.60	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.02	kPa	304.10	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.02	kPa	305.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.03	kPa	307.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.04	kPa	312.60	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.04	kPa	313.40	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

pvap	0.06	kPa	316.60	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.07	kPa	319.70	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.09	kPa	323.20	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.10	kPa	325.20	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.13	kPa	328.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.16	kPa	332.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.17	kPa	333.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.22	kPa	337.00	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.26	kPa	339.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.29	kPa	341.00	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35203442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies	https://www.doi.org/10.1016/j.jct.2011.05.004
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
McGowan Method	
1H-Imidazole:	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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