

1H-Imidazole, 1-pentyl

Other names:	1-pentyl-1H-imidazole 1-pentylimidazole N-pentylimidazole
Inchi:	InChI=1S/C8H14N2/c1-2-3-4-6-10-7-5-9-8-10/h5,7-8H,2-4,6H2,1H3
InchiKey:	UPYVYJSWGZMBOU-UHFFFAOYSA-N
Formula:	C8H14N2
SMILES:	CCCCCn1ccnc1
Mol. weight [g/mol]:	138.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.073		Crippen Method
mcpvol	124.080	ml/mol	McGowan Method
ripol	1258.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1956.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	5.10e-03	kPa	308.20	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	7.75e-03	kPa	313.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.01	kPa	318.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

pvap	0.02	kPa	323.70	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.03	kPa	328.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.03	kPa	333.70	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.05	kPa	338.50	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.09	kPa	345.80	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.10	kPa	348.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.12	kPa	350.70	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.14	kPa	353.20	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.17	kPa	355.90	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.18	kPa	358.10	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

pvap	0.21	kPa	360.80	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.24	kPa	363.10	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles
pvap	0.30	kPa	366.30	Building blocks for ionic liquids: Vapor pressures and vaporization enthalpies of 1-(n-alkyl)-imidazoles

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R68334&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 of 1-(n-alkyl)-imidazoles:	https://www.doi.org/10.1016/j.jct.2011.05.004

Legend

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

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