

1H-Imidazole, 2-methyl-1-pentyl

Other names:	1-pentyl-2-methylimidazole 2-methyl-1-pentyl-1H-imidazole
Inchi:	InChI=1S/C9H16N2/c1-3-4-5-7-11-8-6-10-9(11)2/h6,8H,3-5,7H2,1-2H3
InchiKey:	WYGYPEMNIUDFBC-UHFFFAOYSA-N
Formula:	C9H16N2
SMILES:	CCCCCn1ccnc1C
Mol. weight [g/mol]:	152.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.382		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1972.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	2.66e-03	kPa	303.30	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	3.15e-03	kPa	305.30	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

pvap	3.81e-03	kPa	307.40	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	4.94e-03	kPa	310.40	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	7.00e-03	kPa	314.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	9.29e-03	kPa	317.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.01	kPa	321.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.02	kPa	324.30	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.02	kPa	326.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

pvap	0.02	kPa	327.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.02	kPa	328.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.03	kPa	331.30	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.03	kPa	332.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.03	kPa	334.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.04	kPa	335.30	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.05	kPa	339.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

pvap	0.05	kPa	339.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.06	kPa	343.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.07	kPa	346.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.09	kPa	348.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.09	kPa	349.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.10	kPa	350.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.11	kPa	351.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

pvap	0.12	kPa	352.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.12	kPa	353.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.13	kPa	354.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles :	https://www.doi.org/10.1021/je200336c
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R68348&Units=SI

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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