1H-Imidazole, 1-butyl-2-methyl

Other names: 1-butyl-2-methyl-1H-imidazole
1-butyl-2-methylimidazole
Inchi: InChI=1S/C8H14N2/c1-3-4-6-10-7-5-9-8(10)2/h5,7H,3-4,6H2,1-2H3
InchiKey: WHLZPGRDRYCVRQ-UHFFFAOYSA-N
Formula: C8H14N2
SMILES: CCCCn1ccnc1C
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	1.992		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1876.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	2.35e-03	kPa	293.60	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	2.92e-03	kPa	296.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

pvap	3.44e-03	kPa	298.20	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	4.30e-03	kPa	300.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	5.47e-03	kPa	303.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	6.51e-03	kPa	305.10	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	7.72e-03	kPa	307.20	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	310.20	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	311.10	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	313.20	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	313.20	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	314.10	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	316.10	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	317.10	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	319.10	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	322.10	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	325.10	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	328.10	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	330.10	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	331.10	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	334.00	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.08	kPa	337.00	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles
pvap	0.08	kPa	337.00	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	340.00	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	342.00	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	343.00	Building Blocks for Ionic Liquids: A Study of Alkyl Chain Length Dependence of Vaporization Enthalpies of 1-(n-Alkyl)-2-methylimidazoles

Sources

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=R68281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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