

1H-Imidazole, 1-phenyl-

Other names:	1-phenylimidazole
Inchi:	InChI=1S/C9H8N2/c1-2-4-9(5-3-1)11-7-6-10-8-11/h1-8H
InchiKey:	SEULWJSKCVACTH-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	c1ccc(-n2ccnc2)cc1
Mol. weight [g/mol]:	144.17
CAS:	7164-98-9

Physical Properties

Property code	Value	Unit	Source
hvap	84.60 ± 3.70	kJ/mol	NIST Webbook
log10ws	-2.89		Crippen Method
logp	1.872		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
tb	549.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	4.10e-04	kPa	298.70	Thermochemical properties of different phenyl-1H-imidazoles
pvap	1.05e-03	kPa	308.60	Thermochemical properties of different phenyl-1H-imidazoles
pvap	1.58e-03	kPa	313.50	Thermochemical properties of different phenyl-1H-imidazoles
pvap	2.54e-03	kPa	318.40	Thermochemical properties of different phenyl-1H-imidazoles
pvap	2.69e-03	kPa	319.10	Thermochemical properties of different phenyl-1H-imidazoles

pvap	3.93e-03	kPa	323.50	Thermochemical properties of different phenyl-1H-imidazoles
pvap	5.94e-03	kPa	328.50	Thermochemical properties of different phenyl-1H-imidazoles
pvap	9.02e-03	kPa	333.70	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.01	kPa	338.40	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.02	kPa	343.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.03	kPa	348.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.04	kPa	353.10	Thermochemical properties of different phenyl-1H-imidazoles

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	415.20	K	2.00	NIST Webbook
tbrp	426.70	K	3.10	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7164989&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemical properties of different phenyl-1H-imidazoles: <https://www.doi.org/10.1016/j.fluid.2016.11.010>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_{brp}:	Boiling point at reduced pressure

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