

1-(4-Fluorophenyl)imidazole

Other names:	1-(4-fluorophenyl)-1H-imidazole 4-fluoro-phenyl-1H-imidazole N-(4-fluorophenyl)imidazole
Inchi:	InChI=1S/C9H7FN2/c10-8-1-3-9(4-2-8)12-6-5-11-7-12/h1-7H
InchiKey:	KKKSMWMXKUAZHK-UHFFFAOYSA-N
Formula:	C9H7FN2
SMILES:	Fc1ccc(-n2ccnc2)cc1
Mol. weight [g/mol]:	162.16
CAS:	21441-24-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	2.011		Crippen Method
mcvol	116.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
pvap	1.08e-03	kPa	313.00	Thermochemical properties of different phenyl-1H-imidazoles
pvap	1.66e-03	kPa	318.40	Thermochemical properties of different phenyl-1H-imidazoles
pvap	2.68e-03	kPa	323.30	Thermochemical properties of different phenyl-1H-imidazoles
pvap	4.01e-03	kPa	328.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	5.63e-03	kPa	333.20	Thermochemical properties of different phenyl-1H-imidazoles

pvap	7.02e-03	kPa	335.70	Thermochemical properties of different phenyl-1H-imidazoles
pvap	8.34e-03	kPa	338.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.01	kPa	340.70	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.01	kPa	343.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.01	kPa	345.60	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.02	kPa	348.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.02	kPa	353.10	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.04	kPa	358.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.05	kPa	363.20	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.07	kPa	368.10	Thermochemical properties of different phenyl-1H-imidazoles
pvap	0.09	kPa	373.10	Thermochemical properties of different phenyl-1H-imidazoles

Sources

- 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>
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C21441247&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure

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