

1H-Pyrazole, 1-ethyl-

Other names:	1-Ethylpyrazole
Inchi:	InChI=1S/C5H8N2/c1-2-7-5-3-4-6-7/h3-5H,2H2,1H3
InchiKey:	FLNMQGISZVYIIK-UHFFFAOYSA-N
Formula:	C5H8N2
SMILES:	CCn1cccn1
Mol. weight [g/mol]:	96.13
CAS:	2817-71-2

Physical Properties

Property code	Value	Unit	Source
hvap	53.30 ± 2.40	kJ/mol	NIST Webbook
log10ws	-1.50		Crippen Method
logp	0.903		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	809.00		NIST Webbook
rinpol	809.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2817712&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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