Fomepizole

Other names:	1H-Pyrazole, 4-methyl-
	Pyrazole, 4-methyl-
	4-Methylpyrazol
	4-Methylpyrazole
	4-Methyl-1H-pyrazole
	4-Mp
Inchi:	InChI=1S/C4H6N2/c1-4-2-5-6-3-4/h2-3H,1H3,(H,5,6)
InchiKey:	RIKMMFOAQPJVMX-UHFFFAOYSA-N
Formula:	C4H6N2
SMILES:	Cc1cn[nH]c1
Mol. weight [g/mol]:	82.10
CAS:	7554-65-6

Physical Properties

Property code	Value	Unit	Source
affp	906.80	kJ/mol	NIST Webbook
basg	873.40	kJ/mol	NIST Webbook
log10ws	-0.93		Crippen Method
logp	0.236		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	964.00		NIST Webbook
rinpol	941.00		NIST Webbook
ripol	1929.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.70	K	0.80	NIST Webbook
tbrp	477.70	K	97.30	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7554656&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure