1,2,5-Trimethylpyrrole

Other names: 1H-Pyrrole, 1,2,5-trimethyl-
Pyrrole, 1,2,5-trimethyl
pyrrole, 1,2,5-trimethyl-
Inchi: InChI=1S/C7H11N/c1-6-4-5-7(2)8(6)3/h4-5H,1-3H3
InchiKey: YRABRACUKBOTKB-UHFFFAOYSA-N
Formula: C7H11N
SMILES: Cc1ccc(C)n1C
Mol. weight [g/mol]: 109.17
CAS: 930-87-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	1.642		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
tb	446.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	50.70	kJ/mol	298.15	Experimental and high level ab initio enthalpies of formation of di-, tri- tetra- and pentamethyl-substituted pyrroles

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C930870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and high level ab initio enthalpies of formation of di- tri- tetra- and pentamethyl- substituted pyrroles:	https://www.doi.org/10.1016/j.jct.2014.04.003

Legend

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature