1H-Pyrrole, 2,4-dimethyl-

Other names:	2,4-Dimethyl-1H-pyrrole
	2,4-Dimethylpyrrole
	Pyrrole, 2,4-dimethyl-
Inchi:	InChI=1S/C6H9N/c1-5-3-6(2)7-4-5/h3-4,7H,1-2H3
InchiKey:	MFFMQGGZCLEMCI-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	Cc1c[nH]c(C)c1
Mol. weight [g/mol]:	95.14
CAS:	625-82-1

Physical Properties

Property code	Value	Unit	Source
ie	7.54 ± 0.02	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.150		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
rinpol	842.00		NIST Webbook
sl	222.01	J/mol×K	NIST Webbook
tb	438.45 ± 0.30	K	NIST Webbook
tb	438.45 ± 0.50	K	NIST Webbook
tc	653.00	K	Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results
tf	268.44	K	NIST Webbook
tt	268.44 ± 0.01	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	192.19	J/mol×K	298.15	NIST Webbook

hfust	9.60	kJ/mol	268.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53071e+01
Coeff. B	-4.00465e+03
Coeff. C	-6.37900e+01
Temperature range (K), min.	330.42
Temperature range (K), max.	464.43

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625821&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results:	https://www.doi.org/10.1016/j.jct.2017.09.005

Legend

cpl:	Liquid phase heat capacity
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

tt: Triple Point Temperature