1H-Pyrrole, 2,5-dimethyl-

Other names:	2,5-DIMETHYL-1H-PYRROLE
	2,5-DIMETHYLPYRROLE
	Pyrrole, 2,5-dimethyl-
Inchi:	InChI=1S/C6H9N/c1-5-3-4-6(2)7-5/h3-4,7H,1-2H3
InchiKey:	PAPNRQCYSFBWDI-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	Cc1ccc(C)[nH]1
Mol. weight [g/mol]:	95.14
CAS:	625-84-3

Physical Properties

Property code	Value	Unit	Source
af	0.4460		KDB
affp	918.70	kJ/mol	NIST Webbook
basg	887.10	kJ/mol	NIST Webbook
chl	-3630.50 ± 0.75	kJ/mol	NIST Webbook
hf	39.70 ± 0.88	kJ/mol	NIST Webbook
hfl	-16.80 ± 0.84	kJ/mol	NIST Webbook
hvap	56.50 ± 0.20	kJ/mol	NIST Webbook
hvap	56.50	kJ/mol	NIST Webbook
ie	7.69	eV	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.150		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
pc	5100.00	kPa	KDB
rinpol	900.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	898.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	867.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1601.00		NIST Webbook
ripol	1579.00		NIST Webbook

ripol	1635.00		NIST Webbook
ripol	1590.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1589.00		NIST Webbook
ripol	1589.00		NIST Webbook
sl	212.13	J/mol×K	NIST Webbook
sl	212.13	J/mol×K	NIST Webbook
sl	212.24	J/mol×K	NIST Webbook
tb	405.50	K	KDB
tc	661.00	K	KDB
tc	662.00	K	Thermodynamic properties of pyrrole, 1-methylpyrrole, 2,4-dimethylpyrrole, and 2,5-dimethylpyrrole: Experimental and computational results
tf	280.90	K	NIST Webbook
tt	279.91 ± 0.05	K	NIST Webbook
tt	280.83 ± 0.04	K	NIST Webbook
tt	280.90 ± 0.02	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	195.30	J/mol×K	298.15	NIST Webbook
cpl	195.30	J/mol×K	298.15	NIST Webbook
cpl	195.30	J/mol×K	298.15	NIST Webbook
hfust	9.30	kJ/mol	280.90	NIST Webbook
hfust	9.30	kJ/mol	280.90	NIST Webbook
hfust	9.30	kJ/mol	280.90	NIST Webbook
hfust	9.30	kJ/mol	280.90	NIST Webbook
hvapt	49.50	kJ/mol	208.00	NIST Webbook
sfust	33.10	J/mol×K	280.90	NIST Webbook
sfust	33.09	J/mol×K	280.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.20	K	98.70	NIST Webbook

tbrp	324.70	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57451e+01
Coeff. B	-4.14564e+03
Coeff. C	-6.46240e+01
Temperature range (K), min.	332.82
Temperature range (K), max.	461.96

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1349
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625843&Units=SI

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization 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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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