

1H-Pyrrole, 2,5-dihydro-

Other names:	3-Pyrroline «delta»3-Pyrroline 2,5-Dihydropyrrole Pyrroline 2,5-Dihydro-1H-pyrrole 2,5-dihydro-H-pyrrole
Inchi:	InChI=1S/C4H7N/c1-2-4-5-3-1/h1-2,5H,3-4H2
InchiKey:	JVQIKJMSUIMUDI-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	C1=CCNC1
Mol. weight [g/mol]:	69.11
CAS:	109-96-6

Physical Properties

Property code	Value	Unit	Source
gf	144.73	kJ/mol	Joback Method
hf	50.52	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	32.11	kJ/mol	Joback Method
ie	8.61 ± 0.05	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-0.43		Crippen Method
logp	0.146		Crippen Method
mcvol	62.040	ml/mol	McGowan Method
pc	5670.27	kPa	Joback Method
tb	363.70	K	NIST Webbook
tb	363.65 ± 1.50	K	NIST Webbook
tc	569.87	K	Joback Method
tf	255.77	K	Joback Method
vc	0.225	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	91.48	J/mol×K	358.58	Joback Method
cpg	101.21	J/mol×K	393.80	Joback Method
cpg	110.42	J/mol×K	429.01	Joback Method
cpg	119.11	J/mol×K	464.23	Joback Method
cpg	127.31	J/mol×K	499.44	Joback Method
cpg	135.04	J/mol×K	534.66	Joback Method
cpg	142.31	J/mol×K	569.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.70	K	99.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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