

1-Pyrroline

Other names:	3,4-dihydro-2H-pyrrole 2H-Pyrrole, 3,4-dihydro-
Inchi:	InChI=1S/C4H7N/c1-2-4-5-3-1/h3H,1-2,4H2
InchiKey:	ZVJHJDDKYZXRJI-UHFFFAOYSA-N
Formula:	C4H7N
SMILES:	C1=NCCC1
Mol. weight [g/mol]:	69.11
CAS:	5724-81-2

Physical Properties

Property code	Value	Unit	Source
gf	173.80	kJ/mol	Joback Method
hf	63.00 ± 1.00	kJ/mol	NIST Webbook
hfus	5.34	kJ/mol	Joback Method
hvap	35.00	kJ/mol	NIST Webbook
ie	9.71	eV	NIST Webbook
log10ws	-0.56		Crippen Method
logp	0.851		Crippen Method
mcvol	62.040	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
rinpol	656.00		NIST Webbook
rinpol	656.00		NIST Webbook
rinpol	651.00		NIST Webbook
rinpol	645.00		NIST Webbook
ripol	1021.00		NIST Webbook
ripol	990.00		NIST Webbook
ripol	1021.00		NIST Webbook
tb	363.73	K	Joback Method
tc	580.22	K	Joback Method
tf	222.28	K	Joback Method
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.57	J/mol×K	363.73	Joback Method
cpg	112.11	J/mol×K	399.81	Joback Method
cpg	123.04	J/mol×K	435.89	Joback Method
cpg	133.39	J/mol×K	471.97	Joback Method
cpg	143.15	J/mol×K	508.06	Joback Method
cpg	152.36	J/mol×K	544.14	Joback Method
cpg	161.01	J/mol×K	580.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5724812&Units=SI

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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