

1H-Pyrazole, 3-ethyl-4,5-dihydro-

Other names:	3-Ethyl-«DELTA»[2]-pyrazoline 3-Ethyl-4,5-dihydro-1H-pyrazole
Inchi:	InChI=1S/C5H10N2/c1-2-5-3-4-6-7-5/h6H,2-4H2,1H3
InchiKey:	WYAQEFBMDQTMID-UHFFFAOYSA-N
Formula:	C5H10N2
SMILES:	CCC1=NNCC1
Mol. weight [g/mol]:	98.15
CAS:	5920-29-6

Physical Properties

Property code	Value	Unit	Source
gf	260.30	kJ/mol	Joback Method
hf	89.38	kJ/mol	Joback Method
hfus	17.13	kJ/mol	Joback Method
hvap	41.21	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.746		Crippen Method
mvol	86.110	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
tb	440.14	K	Joback Method
tc	665.06	K	Joback Method
tf	351.10	K	Joback Method
vc	0.330	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.61	J/molxK	440.14	Joback Method
cpg	187.54	J/molxK	477.63	Joback Method
cpg	199.86	J/molxK	515.11	Joback Method
cpg	211.59	J/molxK	552.60	Joback Method
cpg	222.72	J/molxK	590.09	Joback Method
cpg	233.25	J/molxK	627.57	Joback Method
cpg	243.18	J/molxK	665.06	Joback Method

Sources

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=C5920296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
h vap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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