

Oxazole, 4,5-dihydro-2-methyl-

Other names:	2-Methyloxazoline 2-Methyl-2-oxazoline 2-Oxazoline, 2-methyl-
Inchi:	InChI=1S/C4H7NO/c1-4-5-2-3-6-4/h2-3H2,1H3
InchiKey:	GUXJXWKCUUWCLX-UHFFFAOYSA-N
Formula:	C4H7NO
SMILES:	CC1=NCCO1
Mol. weight [g/mol]:	85.10
CAS:	1120-64-5

Physical Properties

Property code	Value	Unit	Source
chl	-2404.90 ± 0.84	kJ/mol	NIST Webbook
gf	78.05	kJ/mol	Joback Method
hf	-130.50 ± 0.92	kJ/mol	NIST Webbook
hfl	-169.50 ± 0.88	kJ/mol	NIST Webbook
hfus	12.93	kJ/mol	Joback Method
hvap	39.10 ± 0.30	kJ/mol	NIST Webbook
h _{vap}	39.10 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.14		Crippen Method
logp	0.435		Crippen Method
m _{cvol}	67.910	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	384.20	K	NIST Webbook
tc	614.46	K	Joback Method
tf	261.37	K	Joback Method
vc	0.258	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.30	J/mol×K	395.66	Joback Method
cpg	138.95	J/mol×K	432.13	Joback Method
cpg	149.10	J/mol×K	468.59	Joback Method

cpg	158.75	J/mol×K	505.06	Joback Method
cpg	167.89	J/mol×K	541.53	Joback Method
cpg	176.55	J/mol×K	577.99	Joback Method
cpg	184.72	J/mol×K	614.46	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=C1120645&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	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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