

Oxazole, 4,5-dihydro-2,4,4-trimethyl-

Other names:	2,4,4-Trimethyl-2-oxazoline 2-Oxazoline, 2,4,4-trimethyl- 2,4,4-Trimethyl-1,3-oxazoline 4,5-Dihydro-2,4,4-trimethyloxazole 2,4,4-Trimethyl-delta ² -oxazoline
Inchi:	InChI=1S/C6H11NO/c1-5-7-6(2,3)4-8-5/h4H2,1-3H3
InchiKey:	HZRZMHNRCISQFT-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	CC1=NC(C)(C)CO1
Mol. weight [g/mol]:	113.16
CAS:	1772-43-6

Physical Properties

Property code	Value	Unit	Source
gf	81.69	kJ/mol	Joback Method
hf	-106.17	kJ/mol	Joback Method
hfus	12.88	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.214		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
tb	385.70	K	NIST Webbook
tc	660.06	K	Joback Method
tf	303.57	K	Joback Method
vc	0.366	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.09	J/molxK	436.99	Joback Method
cpg	220.24	J/molxK	474.17	Joback Method
cpg	233.41	J/molxK	511.35	Joback Method
cpg	245.69	J/molxK	548.53	Joback Method

cpg	257.17	J/mol×K	585.71	Joback Method
cpg	267.95	J/mol×K	622.88	Joback Method
cpg	278.12	J/mol×K	660.06	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=C1772436&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
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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