

2,4,5-Trimethyl-3-oxazoline

Other names:	Oxazole, 2,5-dihydro-2,4,5-trimethyl- 2,4,5-trimethyl-2,5-dihydro-1,3-oxazole
Inchi:	InChI=1S/C6H11NO/c1-4-5(2)8-6(3)7-4/h5-6H,1-3H3
InchiKey:	YFSGRMONVCFYTC-UHFFFAOYSA-N
Formula:	C6H11NO
SMILES:	CC1=NC(C)OC1C
Mol. weight [g/mol]:	113.16
CAS:	22694-96-8

Physical Properties

Property code	Value	Unit	Source
gf	79.47	kJ/mol	Joback Method
hf	-141.75	kJ/mol	Joback Method
hfus	20.25	kJ/mol	Joback Method
hvap	40.57	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.212		Crippen Method
mcvol	96.090	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpola	819.00		NIST Webbook
rinpola	819.00		NIST Webbook
ripola	1124.00		NIST Webbook
ripola	1124.00		NIST Webbook
tb	432.08	K	Joback Method
tc	644.93	K	Joback Method
tf	275.43	K	Joback Method
vc	0.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.96	J/mol×K	432.08	Joback Method
cpg	220.06	J/mol×K	467.56	Joback Method
cpg	233.57	J/mol×K	503.03	Joback Method

cpg	246.50	J/mol×K	538.51	Joback Method
cpg	258.83	J/mol×K	573.98	Joback Method
cpg	270.57	J/mol×K	609.46	Joback Method
cpg	281.70	J/mol×K	644.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22694968&Units=SI
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

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
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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