2-Ethyl-4,4-dimethyl-2-oxazoline

Other names: 4,4-Dimethyl-2-ethyl-2-oxazoline
Oxazole, 2-ethyl-4,5-dihydro-4,4-dimethyl-
2-ethyl-4,5-dihydro-4,4-dimethyloxazole
Inchi: InChI=1S/C7H13NO/c1-4-6-8-7(2,3)5-9-6/h4-5H2,1-3H3
InchiKey: FGURMUFTHTVTAL-UHFFFAOYSA-N
Formula: C7H13NO
SMILES: CCC1=NC(C)(C)CO1
Mol. weight [g/mol]: 127.18
CAS: 5146-88-3

Physical Properties

Property code	Value	Unit	Source
gf	90.11	kJ/mol	Joback Method
hf	-126.81	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	1.604		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	459.87	K	Joback Method
tc	679.72	K	Joback Method
tf	314.84	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.35	J/mol×K	459.87	Joback Method
cpg	262.57	J/mol×K	496.51	Joback Method
cpg	276.79	J/mol×K	533.15	Joback Method
cpg	290.11	J/mol×K	569.80	Joback Method
cpg	302.61	J/mol×K	606.44	Joback Method
cpg	314.39	J/mol×K	643.08	Joback Method

cpg	325.55	J/mol×K	679.72	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=C5146883&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
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