

2-Oxazolanone, 5-methyl-

Other names:	2-Oxazolidinone,5-methyl-
Inchi:	InChI=1S/C4H7NO2/c1-3-2-5-4(6)7-3/h3H,2H2,1H3,(H,5,6)
InchiKey:	HBRXQSHUXIJOKV-UHFFFAOYSA-N
Formula:	C4H7NO2
SMILES:	CC1CN=C(O)O1
Mol. weight [g/mol]:	101.10
CAS:	1072-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-66.48	kJ/mol	Joback Method
hf	-232.36	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	53.11	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	0.319		Crippen Method
mcvol	73.780	ml/mol	McGowan Method
pc	5765.39	kPa	Joback Method
tb	483.17	K	Joback Method
tc	688.72	K	Joback Method
tf	317.95	K	Joback Method
vc	0.276	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.63	J/mol×K	483.17	Joback Method
cpg	181.16	J/mol×K	517.43	Joback Method
cpg	190.24	J/mol×K	551.69	Joback Method
cpg	198.88	J/mol×K	585.95	Joback Method
cpg	207.07	J/mol×K	620.20	Joback Method
cpg	214.81	J/mol×K	654.46	Joback Method
cpg	222.09	J/mol×K	688.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1072704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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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