

5(4H)-Oxazolone, 2-methyl-4-(phenylmethylene)-

Other names:	4-Benzyliden-2-methyl-4,5-dihydro-1,3-oxazol-5-on 4-Benzylidene-2-methyl-4,5-dihydro-1,3-oxazol-5-one 4-Benzylidene-2-methyl-2-oxazolin-5-one 2-Methyl-4-(phenylmethylene)oxazol-5(4H)-one NSC 10132
Inchi:	InChI=1S/C11H9NO2/c1-8-12-10(11(13)14-8)7-9-5-3-2-4-6-9/h2-7H,1H3/b10-7+
InchiKey:	BWQBTJRPSDVWIR-JXMROGBWSA-N
Formula:	C11H9NO2
SMILES:	CC1=NC(=Cc2ccccc2)C(=O)O1
Mol. weight [g/mol]:	187.19
CAS:	881-90-3

Physical Properties

Property code	Value	Unit	Source
gf	172.27	kJ/mol	Joback Method
hf	-29.41	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.003		Crippen Method
mcvol	140.050	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	656.96	K	Joback Method
tc	923.67	K	Joback Method
tf	445.26	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.60	J/molxK	656.96	Joback Method
cpg	379.90	J/molxK	701.41	Joback Method
cpg	393.92	J/molxK	745.86	Joback Method
cpg	406.68	J/molxK	790.32	Joback Method

cpg	418.17	J/mol×K	834.77	Joback Method
cpg	428.40	J/mol×K	879.22	Joback Method
cpg	437.39	J/mol×K	923.67	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=C881903&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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