

2,4-Dimethyl-2-oxazoline-4-methanol

Other names:	2,4-Dimethyl-4-hydroxymethyl-2-oxazoline 4-Oxazolemethanol, 4,5-dihydro-2,4-dimethyl-
Inchi:	InChI=1S/C6H11NO2/c1-5-7-6(2,3-8)4-9-5/h8H,3-4H2,1-2H3
InchiKey:	YWLSGHOSSUXBJK-UHFFFAOYSA-N
Formula:	C6H11NO2
SMILES:	CC1=NC(C)(CO)CO1
Mol. weight [g/mol]:	129.16
CAS:	39986-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-55.13	kJ/mol	Joback Method
hf	-258.40	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	56.41	kJ/mol	Joback Method
log10ws	-0.35		Crippen Method
logp	0.186		Crippen Method
mvol	101.960	ml/mol	McGowan Method
pc	4665.71	kPa	Joback Method
tb	529.17	K	Joback Method
tc	737.11	K	Joback Method
tf	364.39	K	Joback Method
vc	0.386	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.61	J/mol×K	529.17	Joback Method
cpg	267.04	J/mol×K	563.83	Joback Method
cpg	277.79	J/mol×K	598.48	Joback Method
cpg	287.92	J/mol×K	633.14	Joback Method
cpg	297.51	J/mol×K	667.80	Joback Method
cpg	306.66	J/mol×K	702.46	Joback Method
cpg	315.42	J/mol×K	737.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.00 ± 1.00	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39986373&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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