2-Methyl-4,4-dimethylol oxazoline

Inchi: InChI=1S/C6H11NO3/c1-5-7-6(2-8,3-9)4-10-5/h8-9H,2-4H2,1H3
InchiKey: RUILRLCHVAUQDK-UHFFFAOYSA-N
Formula: C6H11NO3
SMILES: CC1=NC(CO)(CO)CO1
Mol. weight [g/mol]: 145.16
CAS: 4271-18-5

Physical Properties

Property code	Value	Unit	Source
gf	-191.95	kJ/mol	Joback Method
hf	-410.63	kJ/mol	Joback Method
hfus	21.06	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	0.39		Crippen Method
logp	-0.842		Crippen Method
mcvol	107.830	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	621.35	K	Joback Method
tc	816.17	K	Joback Method
tf	425.21	K	Joback Method
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.55	J/mol×K	621.35	Joback Method
cpg	310.95	J/mol×K	653.82	Joback Method
cpg	319.90	J/mol×K	686.29	Joback Method
cpg	328.47	J/mol×K	718.76	Joback Method
cpg	336.72	J/mol×K	751.23	Joback Method
cpg	344.73	J/mol×K	783.70	Joback Method
cpg	352.55	J/mol×K	816.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4271185&Units=SI

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