2-Oxazolidinone,4,4-dimethyl-

Other names: 4,4-Dimethyl-2-oxazolidinone
Inchi: InChI=1S/C5H9NO2/c1-5(2)3-8-4(7)6-5/h3H2,1-2H3,(H,6,7)
InchiKey: SYARCRAQWWGZKY-UHFFFAOYSA-N
Formula: C5H9NO2
SMILES: CC1(C)COC(=O)N1
Mol. weight [g/mol]: 115.13
CAS: 26654-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-98.72	kJ/mol	Joback Method
hf	-302.70	kJ/mol	Joback Method
hfus	13.42	kJ/mol	Joback Method
hvap	41.34	kJ/mol	Joback Method
ie	9.80	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	0.505		Crippen Method
mcvol	87.870	ml/mol	McGowan Method
pc	4945.39	kPa	Joback Method
tb	472.64	K	Joback Method
tc	710.14	K	Joback Method
tf	380.73	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.45	J/mol×K	472.64	Joback Method
cpg	202.53	J/mol×K	512.22	Joback Method
cpg	213.88	J/mol×K	551.81	Joback Method
cpg	224.58	J/mol×K	591.39	Joback Method
cpg	234.72	J/mol×K	630.97	Joback Method
cpg	244.38	J/mol×K	670.55	Joback Method
cpg	253.65	J/mol×K	710.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26654397&Units=SI
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

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
ie:	Ionization energy
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