Isoxazolidine

Other names:	Isoxazole, tetrahydro-
	1-Oxa-2-azacyclopentane
	1,2-Oxazolidine
	2-Isoxazolidine
Inchi:	InChI=1S/C3H7NO/c1-2-4-5-3-1/h4H,1-3H2
InchiKey:	CIISBYKBBMFLEZ-UHFFFAOYSA-N
Formula:	C3H7NO
SMILES:	C1CNOC1
Mol. weight [g/mol]:	73.09
CAS:	504-72-3

Physical Properties

Property code	Value	Unit	Source
gf	20.23	kJ/mol	Joback Method
hf	-118.62	kJ/mol	Joback Method
hfus	13.96	kJ/mol	Joback Method
hvap	34.11	kJ/mol	Joback Method
ie	9.57	eV	NIST Webbook
log10ws	-0.24		Crippen Method
logp	-0.089		Crippen Method
mcvol	58.120	ml/mol	McGowan Method
pc	6132.23	kPa	Joback Method
tb	363.49	K	Joback Method
tc	574.99	K	Joback Method
tf	270.31	K	Joback Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.20	J/mol×K	363.49	Joback Method
cpg	103.50	J/mol×K	398.74	Joback Method
cpg	112.34	J/mol×K	433.99	Joback Method
cpg	120.72	J/mol×K	469.24	Joback Method

cpg	128.67	J/mol×K	504.49	Joback Method
cpg	136.19	J/mol×K	539.74	Joback Method
cpg	143.30	J/mol×K	574.99	Joback Method

Sources

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=C504723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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