Oxazolidin-2-one

Other names:	1,3-Oxazolidin-2-one
	2-Oxazolidine
	2-Oxazolidinone
	2-oxazolidone
	Carbamic acid, (2-hydroxyethyl)-, «gamma»-lactone
	Oxazolidone
	dimethylene urethane
Inchi:	InChI=1S/C3H5NO2/c5-3-4-1-2-6-3/h1-2H2,(H,4,5)
InchiKey:	IZXIZTKNFFYFOF-UHFFFAOYSA-N
Formula:	C3H5NO2
SMILES:	O=C1NCCO1
Mol. weight [g/mol]:	87.08
CAS:	497-25-6

Physical Properties

Property code	Value	Unit	Source
gf	-102.36	kJ/mol	Joback Method
hf	-256.32	kJ/mol	Joback Method
hfus	13.47	kJ/mol	Joback Method
hvap	38.35	kJ/mol	Joback Method
ie	10.06	eV	NIST Webbook
ie	10.21	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
log10ws	-2.73e-03		Crippen Method
logp	-0.274		Crippen Method
mcvol	59.690	ml/mol	McGowan Method
pc	6482.71	kPa	Joback Method
tb	431.31	K	Joback Method
tc	665.97	K	Joback Method
tf	338.53	K	Joback Method
vc	0.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.01	J/mol×K	626.86	Joback Method
cpg	111.85	J/mol×K	431.31	Joback Method
cpg	120.49	J/mol×K	470.42	Joback Method
cpg	128.84	J/mol×K	509.53	Joback Method
cpg	136.90	J/mol×K	548.64	Joback Method
cpg	144.63	J/mol×K	587.75	Joback Method
cpg	159.02	J/mol×K	665.97	Joback Method
hfust	17.30	kJ/mol	360.00	NIST Webbook
hvapt	83.18	kJ/mol	334.15	Thermochemical and theoretical study of 2-oxazolidinone and 3-acetyl-2-oxazolidinone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.20	K	6.40	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C497256&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemical and theoretical study of 2-oxazolidinone and 3-acetyl-2-oxazolidinone: https://www.doi.org/10.1016/j.jct.2016.07.038

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

hfust: Enthalpy of fusion at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume