Isoxazole

Other names:	1-OXA-2-AZACYCLOPENTADIENE
	Isooxazole
Inchi:	InChI=1S/C3H3NO/c1-2-4-5-3-1/h1-3H
InchiKey:	CTAPFRYPJLPFDF-UHFFFAOYSA-N
Formula:	C3H3NO
SMILES:	c1cnoc1
Mol. weight [g/mol]:	69.06
CAS:	288-14-2

Physical Properties

Property code	Value	Unit	Source
affp	848.60	kJ/mol	NIST Webbook
basg	816.80	kJ/mol	NIST Webbook
chl	-1651.40 ± 0.50	kJ/mol	NIST Webbook
chl	-1654.05 ± 0.32	kJ/mol	NIST Webbook
dm	2.80	debye	KDB
hf	78.58 ± 0.54	kJ/mol	NIST Webbook
hf	82.00 ± 0.60	kJ/mol	NIST Webbook
hfl	44.78 ± 0.56	kJ/mol	NIST Webbook
hfl	42.13 ± 0.54	kJ/mol	NIST Webbook
hvap	37.20 ± 0.20	kJ/mol	NIST Webbook
hvap	36.40 ± 0.04	kJ/mol	NIST Webbook
hvap	37.24 ± 0.22	kJ/mol	NIST Webbook
hvap	36.50 ± 0.10	kJ/mol	NIST Webbook
ie	9.93 ± 0.05	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
ie	9.99 ± 0.05	eV	NIST Webbook
ie	10.20	eV	NIST Webbook
log10ws	-4.97		Crippen Method
logp	0.675		Crippen Method
mcvol	49.520	ml/mol	McGowan Method
pc	6100.00 ± 400.00	kPa	NIST Webbook
rhoc	361.68 ± 20.03	kg/m3	NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	590.00		NIST Webbook
tb	368.70	K	NIST Webbook

tb	367.20	K	NIST Webbook
tb	368.00	K	KDB
tc	552.00	K	KDB
tc	590.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	108.10	J/mol×K	298.15	NIST Webbook
rhol	1078.00	kg/m3	293.00	KDB

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C288142&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
KDB: https://www.cheric.org/files/research/kdb/mol/mol1462.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
cpl: Liquid phase heat capacity
dm: Dipole Moment
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation 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
rhoc: Critical density

rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature