Oxazole

Other names: 1,3-OXAZOLE
Inchi: InChI=1S/C3H3NO/c1-2-5-3-4-1/h1-3H
InchiKey: ZCQWOFVYLHDMMC-UHFFFAOYSA-N
Formula: C3H3NO
SMILES: c1cocn1
Mol. weight [g/mol]: 69.06
CAS: 288-42-6

Physical Properties

Property code	Value	Unit	Source
affp	876.40	kJ/mol	NIST Webbook
basg	844.50	kJ/mol	NIST Webbook
chl	-1561.30 ± 0.50	kJ/mol	NIST Webbook
hf	-15.50 ± 0.54	kJ/mol	NIST Webbook
hfl	-48.03 ± 0.54	kJ/mol	NIST Webbook
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
hvap	32.50 ± 0.10	kJ/mol	NIST Webbook
ie	10.15	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
log10ws	-4.97		Crippen Method
logp	0.675		Crippen Method
mcvol	49.520	ml/mol	McGowan Method
pc	6770.00	kPa	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
rinpol	580.00		NIST Webbook
rinpol	97.30		NIST Webbook
rinpol	97.30		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	580.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	580.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1019.00		NIST Webbook
ripol	1019.00		NIST Webbook

tb	342.71 ± 0.20	K	NIST Webbook
tb	342.70	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	34.60	kJ/mol	318.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47512e+01
Coeff. B	-3.11216e+03
Coeff. C	-3.55670e+01
Temperature range (K), min.	250.74
Temperature range (K), max.	365.25

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060269j
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1461.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C288426&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp: Proton affinity

basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature