Benzoxazole

Other names:	1-Oxa-3-aza-1H-indene
	1-Oxa-3-azaindene
	USAF ek-5017
Inchi:	InChI=1S/C7H5NO/c1-2-4-7-6(3-1)8-5-9-7/h1-5H
InchiKey:	BCMCBBGGLRIHSE-UHFFFAOYSA-N
Formula:	C7H5NO
SMILES:	c1ccc2ocnc2c1
Mol. weight [g/mol]:	119.12
CAS:	273-53-0

Physical Properties

Property code	Value	Unit	Source
affp	891.60	kJ/mol	NIST Webbook
basg	859.80	kJ/mol	NIST Webbook
chs	-3445.00 ± 1.00	kJ/mol	NIST Webbook
hf	45.14 ± 0.52	kJ/mol	NIST Webbook
hfs	-24.20 ± 1.10	kJ/mol	NIST Webbook
hsub	69.50 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.16		Aqueous Solubility Prediction Method
log10ws	-1.16		Estimated Solubility Method
logp	1.828		Crippen Method
mcvol	86.420	ml/mol	McGowan Method
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
ripol	1733.00		NIST Webbook
ripol	1733.00		NIST Webbook
ss	148.95	J/mol×K	NIST Webbook
tb	455.70	K	NIST Webbook
tb	456.00	K	NIST Webbook
tb	456.00	K	NIST Webbook
tf	304.00	K	NIST Webbook
tf	303.65	K	Aqueous Solubility Prediction Method
tt	302.50 ± 0.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	141.59	J/mol×K	298.15	NIST Webbook
hfust	16.78	kJ/mol	302.50	NIST Webbook
hvapt	51.20	kJ/mol	320.00	NIST Webbook
hvapt	48.60	kJ/mol	360.00	NIST Webbook
hvapt	46.10	kJ/mol	400.00	NIST Webbook
hvapt	43.50	kJ/mol	440.00	NIST Webbook
hvapt	40.70	kJ/mol	480.00	NIST Webbook
hvapt	69.20	kJ/mol	298.15	Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxadole derivatives

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C273530&Units=SI

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

Experimental and computational thermochemical studies of benzoxazole and two chlorobenzoxadole derivatives: https://www.doi.org/10.1016/j.jct.2012.08.028

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

affp: Proton affinity

basg: Gas basicity

chs: Standard solid enthalpy of combustion

cps: Solid phase heat capacity

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfust: Enthalpy of fusion at a given temperature

hsub: Enthalpy of sublimation at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature