Benzothiazole, 2-methyl-

Other names:	2-Methylbenzothiazole
	2-methyl-1,3-benzothiazole
	2-methylbenzo[d]thiazole
	USAF ek-1853
Inchi:	InChI=1S/C8H7NS/c1-6-9-7-4-2-3-5-8(7)10-6/h2-5H,1H3
InchiKey:	DXYYSGDWQCSKKO-UHFFFAOYSA-N
Formula:	C8H7NS
SMILES:	Cc1nc2ccccc2s1
Mol. weight [g/mol]:	149.21
CAS:	120-75-2

Physical Properties

Property code	Value	Unit	Source
ie	8.65	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.605		Crippen Method
mcvol	110.990	ml/mol	McGowan Method
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1273.00		NIST Webbook
tb	511.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	61.70	kJ/mol	298.15	Energetic study of benzothiazole and two methylbenzothiazole derivatives: Calorimetric and computational approaches
hvapt	61.30	kJ/mol	421.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79319e+01
Coeff. B	-6.51965e+03
Coeff. C	-2.14500e+01
Temperature range (K), min.	390.95
Temperature range (K), max.	538.05

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Energetic study of benzothiazole and two methylbenzothiazole derivatives: Calorimetric and computational approaches:	https://www.doi.org/10.1016/j.jct.2013.06.021
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120752&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
pvap:	Vapor pressure

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure