Benzothiazole, 2,5-dimethyl-

Other names:	2,5-Dimethylbenzthiazol
	2,5-dimethyl-1,3-benzothiazole
	2,5-dimethylbenzothiazole
Inchi:	InChI=1S/C9H9NS/c1-6-3-4-9-8(5-6)10-7(2)11-9/h3-5H,1-2H3
InchiKey:	XHANCLXYCNTZMM-UHFFFAOYSA-N
Formula:	C9H9NS
SMILES:	Cc1ccc2sc(C)nc2c1
Mol. weight [g/mol]:	163.24
CAS:	95-26-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	2.913		Crippen Method
mcvol	125.080	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	84.90	kJ/mol	298.15	Energetic study of benzothiazole and two methylbenzothiazole derivatives: Calorimetric and computational approaches

Sources

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=C95261&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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