Benzothiazole, 2-phenyl-

Other names:	2-phenylbenzo[d]thiazole
	2-phenylbenzothiazole
Inchi:	InChI=1S/C13H9NS/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H
InchiKey:	XBHOUXSGHYZCNH-UHFFFAOYSA-N
Formula:	C13H9NS
SMILES:	c1ccc(-c2nc3ccccc3s2)cc1
Mol. weight [g/mol]:	211.28
CAS:	883-93-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	3.963		Crippen Method
mcvol	157.680	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	99.30	kJ/mol	298.15	Thermochemical and conformational study of optical active phenylbenzazole derivatives

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical and conformational study of optical active phenylbenzazole derivatives:	https://www.doi.org/10.1016/j.jct.2017.08.017
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C883932&Units=SI

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