Aminothiazole

Other names:	2-Amino-1,3-thiazole
	2-Aminothiazole
	2-Thiazolamine
	2-Thiazolylamine
	4-Thiazolin-2-onimine
	Abadol
	Abadole
	Basedol
	NSC 1900
	RP 2921
	Thiazole, 2-amino-
	USAF EK-P-5501
Inchi:	InChI=1S/C3H4N2S/c4-3-5-1-2-6-3/h1-2H,(H2,4,5)
InchiKey:	RAIPHJJURHTUIC-UHFFFAOYSA-N
Formula:	C3H4N2S
SMILES:	Nc1nccs1
Mol. weight [g/mol]:	100.14
CAS:	96-50-4

Physical Properties

Property code	Value	Unit	Source
affp	930.60	kJ/mol	NIST Webbook
basg	898.70	kJ/mol	NIST Webbook
log10ws	-0.36		Aqueous Solubility Prediction Method
log10ws	-0.36		Estimated Solubility Method
logp	0.725		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
tf	364.65	K	Aqueous Solubility Prediction Method
tf	363.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	85.90	kJ/mol	298.15	Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	1.50	NIST Webbook
tbrp	413.00	K	1.50	NIST Webbook

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96504&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches:	https://www.doi.org/10.1016/j.jct.2014.04.001
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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