

# Benzothiazole

<b>Other names:</b>	1-Thia-3-azaindene Benzosulfonazole Benzothiazol USAF ek-4812 Vangard BT o-2857
<b>Inchi:</b>	InChI=1S/C7H5NS/c1-2-4-7-6(3-1)8-5-9-7/h1-5H
<b>InchiKey:</b>	IOJUPLGTWVMSFF-UHFFFAOYSA-N
<b>Formula:</b>	C7H5NS
<b>SMILES:</b>	<chem>c1ccc2scnc2c1</chem>
<b>Mol. weight [g/mol]:</b>	135.19
<b>CAS:</b>	95-16-9

## Physical Properties

Property code	Value	Unit	Source
chl	-4215.15 ± 0.56	kJ/mol	NIST Webbook
hf	204.17 ± 0.37	kJ/mol	NIST Webbook
hfl	144.03 ± 0.70	kJ/mol	NIST Webbook
hsub	72.90 ± 0.60	kJ/mol	NIST Webbook
hvap	60.14	kJ/mol	NIST Webbook
ie	8.65	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
ie	8.72 ± 0.05	eV	NIST Webbook
log10ws	-1.50		Estimated Solubility Method
log10ws	-1.50		Aqueous Solubility Prediction Method
logp	2.296		Crippen Method
mvol	96.900	ml/mol	McGowan Method
rinpol	1221.00		NIST Webbook
rinpol	1269.00		NIST Webbook
rinpol	1207.90		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1196.00		NIST Webbook

rinpol	1221.00	NIST Webbook
rinpol	1258.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1220.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1241.00	NIST Webbook
rinpol	1248.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1225.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1199.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1183.50	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1236.00	NIST Webbook
rinpol	1180.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1184.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1183.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1193.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1216.00	NIST Webbook
rinpol	1244.00	NIST Webbook
rinpol	1245.00	NIST Webbook

rinpol	1223.00	NIST Webbook
rinpol	1231.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1230.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1234.00	NIST Webbook
rinpol	1185.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1228.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1190.00	NIST Webbook
rinpol	1216.00	NIST Webbook
rinpol	1254.00	NIST Webbook
rinpol	1246.00	NIST Webbook
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rinpol	1243.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1245.00	NIST Webbook
rinpol	1186.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1198.00	NIST Webbook
rinpol	1190.00	NIST Webbook
rinpol	1178.00	NIST Webbook
rinpol	207.39	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1226.00	NIST Webbook
rinpol	1222.00	NIST Webbook
rinpol	1201.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1243.00	NIST Webbook
rinpol	1244.30	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1223.00	NIST Webbook
rinpol	1221.00	NIST Webbook
rinpol	1267.00	NIST Webbook
rinpol	1246.00	NIST Webbook
rinpol	1218.00	NIST Webbook
rinpol	1227.00	NIST Webbook
rinpol	1190.00	NIST Webbook
rinpol	1187.00	NIST Webbook
rinpol	1224.00	NIST Webbook
rinpol	1207.00	NIST Webbook

ripol	1202.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1223.00	NIST Webbook
ripol	1958.00	NIST Webbook
ripol	1948.00	NIST Webbook
ripol	1929.00	NIST Webbook
ripol	1937.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	1982.00	NIST Webbook
ripol	1958.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	1932.00	NIST Webbook
ripol	1961.00	NIST Webbook
ripol	1984.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1991.00	NIST Webbook
ripol	1947.00	NIST Webbook
ripol	2000.00	NIST Webbook
ripol	2002.00	NIST Webbook
ripol	1937.00	NIST Webbook
ripol	1973.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1970.00	NIST Webbook
ripol	1959.00	NIST Webbook
ripol	1965.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1969.00	NIST Webbook
ripol	1996.00	NIST Webbook
ripol	1953.00	NIST Webbook
ripol	1984.00	NIST Webbook
ripol	1942.00	NIST Webbook
ripol	1947.00	NIST Webbook
ripol	1955.00	NIST Webbook
ripol	1952.00	NIST Webbook
ripol	1962.00	NIST Webbook
ripol	1968.00	NIST Webbook
ripol	1951.00	NIST Webbook
ripol	1951.00	NIST Webbook
ripol	1951.00	NIST Webbook
ripol	1936.00	NIST Webbook
ripol	1937.00	NIST Webbook
ripol	1950.00	NIST Webbook
ripol	1912.00	NIST Webbook

ripol	1955.00		NIST Webbook
ripol	1937.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1996.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1995.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1953.00		NIST Webbook
ripol	1942.00		NIST Webbook
ripol	1984.00		NIST Webbook
sl	209.83	J/molxK	NIST Webbook
sl	209.83	J/molxK	NIST Webbook
sl	209.88	J/molxK	NIST Webbook
tb	497.00 ± 1.00	K	NIST Webbook
tb	504.20	K	NIST Webbook
tf	273.88 ± 0.35	K	NIST Webbook
tf	276.05 ± 0.20	K	NIST Webbook
tf	274.95 ± 0.25	K	NIST Webbook
tf	275.29 ± 0.35	K	NIST Webbook
tt	275.65 ± 0.00	K	NIST Webbook
tt	275.60 ± 0.01	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	189.25	J/molxK	298.15	NIST Webbook
cpl	189.54	J/molxK	298.15	NIST Webbook
cpl	189.54	J/molxK	298.15	NIST Webbook
hfust	12.78	kJ/mol	275.60	NIST Webbook
hfust	12.78	kJ/mol	275.60	NIST Webbook
hfust	11.95	kJ/mol	275.50	NIST Webbook
hfust	12.80	kJ/mol	275.60	NIST Webbook
hfust	12.80	kJ/mol	275.60	NIST Webbook
hvapt	58.80	kJ/mol	298.15	Energetic study of benzothiazole and two methylbenzothiazole derivatives: Calorimetric and computational approaches



<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature

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