Benzo[b]thiophene

Other names:	1-Benzothiophene
	1-Thiaindene
	2,3-Benzothiophene
	BENZOTHIOFURAN
	Benzothiophen
	Benzothiophene
	NSC 47196
	THIANAPHTHENE
	THIONAPHTHALENE
	Thianaphtene
	Thianaphthen
	Thionaphthene
Inchi:	InChI=1S/C8H6S/c1-2-4-8-7(3-1)5-6-9-8/h1-6H
InchiKey:	FCEHBMOGCRZNNI-UHFFFAOYSA-N
Formula:	C8H6S
SMILES:	c1ccc2sccc2c1
Mol. weight [g/mol]:	134.20
CAS:	95-15-8

Physical Properties

Property code	Value	Unit	Source
chs	-4708.21 ± 0.79	kJ/mol	NIST Webbook
hf	166.28 ± 0.48	kJ/mol	NIST Webbook
hf	166.60	kJ/mol	NIST Webbook
hfs	100.60 ± 0.45	kJ/mol	NIST Webbook
hfs	100.90 ± 0.92	kJ/mol	NIST Webbook
hsub	65.70	kJ/mol	NIST Webbook
hsub	65.70 ± 0.20	kJ/mol	NIST Webbook
hsub	65.68 ± 0.17	kJ/mol	NIST Webbook
ie	8.73 ± 0.05	eV	NIST Webbook
ie	8.17 ± 0.05	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	8.17 ± 0.03	eV	NIST Webbook
ie	8.13 ± 0.01	eV	NIST Webbook
log10ws	-3.03		Crippen Method
logp	2.901		Crippen Method
mcvol	101.010	ml/mol	McGowan Method

rinpol	1189.00	NIST Webbook
rinpol	201.50	NIST Webbook
rinpol	201.47	NIST Webbook
rinpol	201.50	NIST Webbook
rinpol	201.57	NIST Webbook
rinpol	201.43	NIST Webbook
rinpol	200.51	NIST Webbook
rinpol	201.50	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1180.50	NIST Webbook
rinpol	1188.30	NIST Webbook
rinpol	1192.90	NIST Webbook
rinpol	1180.50	NIST Webbook
rinpol	1188.30	NIST Webbook
rinpol	1192.90	NIST Webbook
rinpol	1195.00	NIST Webbook
rinpol	1155.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1205.00	NIST Webbook
rinpol	1165.00	NIST Webbook
rinpol	1169.00	NIST Webbook
rinpol	1172.00	NIST Webbook
rinpol	1145.00	NIST Webbook
rinpol	1159.00	NIST Webbook
rinpol	1168.00	NIST Webbook
rinpol	1194.00	NIST Webbook
rinpol	1196.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1161.00	NIST Webbook
rinpol	1200.00	NIST Webbook
rinpol	201.57	NIST Webbook
rinpol	200.92	NIST Webbook
rinpol	201.34	NIST Webbook
rinpol	201.29	NIST Webbook
rinpol	201.60	NIST Webbook
rinpol	201.84	NIST Webbook
rinpol	201.44	NIST Webbook
ripol	1751.00	NIST Webbook
ripol	1751.00	NIST Webbook
ripol	1751.00	NIST Webbook

ripol	207.63		NIST Webbook
ripol	1799.00		NIST Webbook
ss	177.11	J/mol×K	NIST Webbook
tb	494.50 ± 0.50	K	NIST Webbook
tb	494.15 ± 0.50	K	NIST Webbook
tb	493.10 ± 0.40	K	NIST Webbook
tb	494.20	K	NIST Webbook
tf	304.47	K	KDB
tf	305.00	K	NIST Webbook
tf	304.49 ± 0.05	K	NIST Webbook
tt	304.48 ± 0.02	K	NIST Webbook
tt	304.50 ± 0.05	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	163.01	J/mol×K	298.15	NIST Webbook
cps	172.14	J/mol×K	295.86	NIST Webbook
hfust	11.84	kJ/mol	304.50	NIST Webbook
hfust	11.83	kJ/mol	304.50	NIST Webbook
hvapt	52.00	kJ/mol	426.00	NIST Webbook
hvapt	49.70	kJ/mol	426.00	NIST Webbook
hvapt	46.20	kJ/mol	426.00	NIST Webbook
hvapt	43.80	kJ/mol	426.00	NIST Webbook
hvapt	54.30	kJ/mol	426.00	NIST Webbook
hvapt	53.80	kJ/mol	326.00	NIST Webbook
hvapt	47.20	kJ/mol	425.00	NIST Webbook
hvapt	42.80	kJ/mol	505.00	NIST Webbook
hvapt	36.10	kJ/mol	605.00	NIST Webbook
hvapt	45.00	kJ/mol	564.50	NIST Webbook
hvapt	47.90	kJ/mol	461.00	NIST Webbook
hvapt	41.20	kJ/mol	426.00	NIST Webbook
hvapt	52.10	kJ/mol	386.50	NIST Webbook
pvap	60.50	kPa	472.44	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	71.50	kPa	479.15	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene

pvap	80.50	kPa	484.01	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	90.90	kPa	489.09	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	101.50	kPa	493.80	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	21.30	kPa	434.26	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	30.30	kPa	446.75	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	41.10	kPa	457.64	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
pvap	50.80	kPa	465.61	Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene
rfi	1.63800		310.15	Separation of sulfur compounds from alkanes with 1-alkylcyanopyridinium-based ionic liquids
rhol	1141.83	kg/m3	318.15	Extraction desulfurization process of fuels with ionic liquids
rhol	1132.85	kg/m3	328.15	Extraction desulfurization process of fuels with ionic liquids

rhol	1150.55	kg/m3	308.15	Phase equilibria study of binary systems comprising an (ionic liquid + hydrocarbon)
rhol	1427.00	kg/m3	298.15	Effect of the alkyl side chain of the 1-alkylpiperidinium-based ionic liquids on desulfurization of fuels
rhol	1150.81	kg/m3	308.15	Extraction desulfurization process of fuels with ionic liquids
sfust	38.84	J/mol×K	304.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	377.20	K	2.70	NIST Webbook
tbrp	377.00 ± 1.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55204e+01
Coeff. B	-4.58245e+03
Coeff. C	-6.01570e+01
Temperature range (K), min.	360.98
Temperature range (K), max.	509.02

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.41625e+01
Coeff. B	-9.41664e+03
Coeff. C	-9.91030e+00

Coeff. D	4.07407e-06
Temperature range (K), min.	304.50
Temperature range (K), max.	754.00

Sources

Experimental Densities of Hexane + Benzothiophene Mixtures from (313 to 368) K and up to 20 MPa:	https://www.doi.org/10.1021/je7003929
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Separation of sulfur compounds from alkanes with 1-alkylcyanopyridinium-based ionic liquids:	https://www.doi.org/10.1016/j.jct.2013.09.032
Liquid-liquid extraction of sulfur compounds from heptane with tricyanomethanide based ionic liquids:	https://www.doi.org/10.1016/j.jct.2018.10.009
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Phase equilibria study of binary systems comprising an (ionic liquid + hydrocarbon):	https://www.doi.org/10.1016/j.jct.2014.12.005
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1855
Ternary liquid-liquid equilibria of trifluorotris(perfluoroethyl)phosphate based ionic liquids + benzothiophene + heptane:	https://www.doi.org/10.1016/j.fluid.2013.10.028
Solvent extraction of aromatic sulfur compounds from n-heptane using the 1-ethyl-3-methylimidazolium tricyanomethanide ionic liquid:	https://www.doi.org/10.1016/j.jct.2013.05.048
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1855.mol
Infinite Dilution Binary Diffusion Coefficients of Hydrotreating Compounds in Tetradecane in the Temperature Range from (310 to 475) K:	https://www.doi.org/10.1021/je700535q
Extraction desulfurization process of fuels with ionic liquids:	https://www.doi.org/10.1016/j.jct.2014.04.025
Separation of thiophene, or benzothiophene from model fuel using glycols. Liquid-liquid phase equilibria and oxidative desulfurization study:	https://www.doi.org/10.1016/j.fluid.2018.10.017
Vapor-Liquid Equilibria of Binary and Ternary Systems Containing Carbon Dioxide, Alkane, and Benzothiophene:	https://www.doi.org/10.1021/je200586g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurements and prediction of ternary liquid-liquid equilibria for mixtures ORL + sulfur compound + dodecane:	https://www.doi.org/10.1016/j.fluid.2016.03.014
Isobaric vapor-liquid equilibrium for binary systems containing benzothiophene:	https://www.doi.org/10.1016/j.fluid.2011.04.024
Effect of the alkyl side chain of the 1-alkylpiperidinium-based ionic liquids on desulfurization of fuels:	https://www.doi.org/10.1016/j.jct.2013.12.029
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95158&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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