Dibenzothiophene

Other names:	2,2'-Biphenylylene sulfide
	9-Thiafluorene
	Dibenzo[b,d]thiophene
	Diphenylene sulfide
	[1,1'-Biphenyl]-2,2'-diyl sulfide
	«alpha»-Thiafluorene
	Â«alphaÂ»-Thiafluorene
Inchi:	InChI=1S/C12H8S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1-8H
InchiKey:	IYYZUPMFVPLQIF-UHFFFAOYSA-N
Formula:	C12H8S
SMILES:	c1ccc2c(c1)sc1ccccc12
Mol. weight [g/mol]:	184.26
CAS:	132-65-0

Physical Properties

Property code	Value	Unit	Source
chs	-6587.70 ± 1.30	kJ/mol	NIST Webbook
chs	-6571.60 ± 4.40	kJ/mol	NIST Webbook
hf	189.30 ± 4.50	kJ/mol	NIST Webbook
hf	205.40	kJ/mol	NIST Webbook
hf	213.20 ± 0.70	kJ/mol	NIST Webbook
hfs	120.30 ± 1.50	kJ/mol	NIST Webbook
hfs	104.20 ± 4.50	kJ/mol	NIST Webbook
hsub	97.50	kJ/mol	NIST Webbook
hsub	85.10 ± 0.40	kJ/mol	NIST Webbook
hsub	93.20 ± 0.50	kJ/mol	NIST Webbook
hsub	85.09 ± 0.35	kJ/mol	NIST Webbook
hsub	85.10	kJ/mol	NIST Webbook
hsub	93.30	kJ/mol	NIST Webbook
hvap	78.30 ± 1.10	kJ/mol	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
ie	8.23	eV	NIST Webbook
ie	7.90 ± 0.03	eV	NIST Webbook
ie	8.01	eV	NIST Webbook
ie	8.14	eV	NIST Webbook
ie	8.44	eV	NIST Webbook

log10ws	-4.38		Estimated Solubility Method
log10ws	-4.62		Aqueous Solubility Prediction Method
logp	4.054		Crippen Method
mcvol	137.910	ml/mol	McGowan Method
rinpol	1719.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1774.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1721.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	295.47		NIST Webbook
rinpol	295.99		NIST Webbook
rinpol	296.06		NIST Webbook
rinpol	295.59		NIST Webbook
rinpol	295.59		NIST Webbook
rinpol	295.73		NIST Webbook
rinpol	295.85		NIST Webbook
rinpol	295.60		NIST Webbook
rinpol	295.60		NIST Webbook
rinpol	296.01		NIST Webbook
rinpol	295.77		NIST Webbook
rinpol	295.78		NIST Webbook
rinpol	295.96		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	295.90		NIST Webbook
rinpol	295.95		NIST Webbook
rinpol	295.40		NIST Webbook
rinpol	295.59		NIST Webbook
rinpol	295.90		NIST Webbook
rinpol	296.03		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	295.31		NIST Webbook
rinpol	296.00		NIST Webbook
rinpol	295.39		NIST Webbook
rinpol	296.01		NIST Webbook
rinpol	295.81		NIST Webbook
rinpol	296.00		NIST Webbook
rinpol	295.95		NIST Webbook
rinpol	295.59		NIST Webbook
rinpol	295.95		NIST Webbook

rinpol	295.70		NIST Webbook
rinpol	295.70		NIST Webbook
rinpol	294.65		NIST Webbook
rinpol	293.59		NIST Webbook
rinpol	295.70		NIST Webbook
rinpol	295.28		NIST Webbook
rinpol	295.24		NIST Webbook
rinpol	295.20		NIST Webbook
rinpol	295.80		NIST Webbook
rinpol	295.90		NIST Webbook
rinpol	295.90		NIST Webbook
rinpol	294.90		NIST Webbook
rinpol	295.90		NIST Webbook
rinpol	295.81		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	295.47		NIST Webbook
rinpol	295.73		NIST Webbook
rinpol	295.77		NIST Webbook
rinpol	1722.00		NIST Webbook
rinpol	294.74		NIST Webbook
rinpol	295.81		NIST Webbook
rinpol	1741.90		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1741.90		NIST Webbook
rinpol	1739.80		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	296.30		NIST Webbook
rinpol	294.74		NIST Webbook
rinpol	295.95		NIST Webbook
ripol	295.17		NIST Webbook
ss	204.20	J/mol×K	NIST Webbook
tb	605.70	K	NIST Webbook
tf	372.00 ± 2.00	K	NIST Webbook
tf	373.15	K	Thermodynamic models for determination of the solubility of dibenzothiophene in (methanol + acetonitrile) binary solvent mixtures

tf	373.15	K	Thermodynamic Models for Determination of the Solubility of Dibenzothiophene in Different Solvents at Temperatures from (278.15 to 328.15) K
tf	371.90 ± 0.30	K	NIST Webbook
tf	371.40 ± 0.10	K	NIST Webbook
tf	371.00 ± 0.70	K	NIST Webbook
tf	372.40 ± 0.30	K	NIST Webbook
tf	373.00 ± 2.00	K	NIST Webbook
tf	372.00 ± 2.00	K	NIST Webbook
tt	371.82 ± 0.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	194.60	J/mol×K	298.15	NIST Webbook
cps	198.30	J/mol×K	298.15	NIST Webbook
hfust	21.60	kJ/mol	371.80	NIST Webbook
hfust	21.58	kJ/mol	371.00	NIST Webbook
hfust	21.58	kJ/mol	371.00	NIST Webbook
hfust	21.60	kJ/mol	373.20	NIST Webbook
hfust	21.60	kJ/mol	373.20	NIST Webbook
hfust	21.58	kJ/mol	371.00	NIST Webbook
hfust	21.71	kJ/mol	371.82	NIST Webbook
hsubt	90.70	kJ/mol	348.00	NIST Webbook
hsubt	91.20	kJ/mol	325.50	NIST Webbook
hvapt	65.60	kJ/mol	398.50	NIST Webbook
hvapt	66.80 ± 0.30	kJ/mol	420.00	NIST Webbook
hvapt	64.30 ± 0.30	kJ/mol	460.00	NIST Webbook
hvapt	61.80 ± 0.30	kJ/mol	500.00	NIST Webbook
hvapt	59.30 ± 0.30	kJ/mol	540.00	NIST Webbook
hvapt	69.50 ± 0.30	kJ/mol	380.00	NIST Webbook
hvapt	54.00 ± 0.30	kJ/mol	620.00	NIST Webbook
hvapt	68.00 ± 0.10	kJ/mol	518.50	NIST Webbook
hvapt	64.90 ± 0.10	kJ/mol	518.50	NIST Webbook
hvapt	61.80 ± 0.10	kJ/mol	518.50	NIST Webbook
hvapt	58.70 ± 0.10	kJ/mol	518.50	NIST Webbook
hvapt	55.40 ± 0.30	kJ/mol	518.50	NIST Webbook
hvapt	51.80 ± 0.40	kJ/mol	518.50	NIST Webbook
hvapt	60.10	kJ/mol	479.50	NIST Webbook

hvapt	56.90	kJ/mol	590.00	NIST Webbook
hvapt	55.30	kJ/mol	610.00	NIST Webbook
hvapt	53.60	kJ/mol	630.00	NIST Webbook
hvapt	69.40	kJ/mol	388.00	NIST Webbook
hvapt	63.40	kJ/mol	516.00	NIST Webbook
hvapt	56.80 ± 0.30	kJ/mol	580.00	NIST Webbook
sfust	58.17	J/mol×K	371.00	NIST Webbook
sfust	58.38	J/mol×K	371.82	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.20	K	0.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.73523e+01
Coeff. B	-7.78795e+03
Coeff. C	5.89000e+00
Temperature range (K), min.	424.00
Temperature range (K), max.	640.91

Sources

Infinite Dilution Binary Diffusion Coefficients of Hydrotreating Compounds in n-Tetradecane in the Temperature Range from (310 to 475) K:	https://www.doi.org/10.1021/je700535q
Solid–Liquid Equilibria of Dibenzothiophene and Dibenzothiophene Sulfone in Organic Solvents:	https://www.doi.org/10.1021/je700234e
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solubility of dibenzothiophene in nine organic solvents: Experimental measurement and thermodynamic modeling:	https://www.doi.org/10.1016/j.jct.2018.09.017
Feasibility of phosphonium-based ionic liquids as solvents for extractive desulfurization of liquid fuels:	https://www.doi.org/10.1016/j.fluid.2015.05.015
Thermodynamic Models for Determination of the Solubility of Dibenzothiophene in Different Solvents at Temperatures from 274.15 to 328.15) K:	https://www.doi.org/10.1021/je500437m
Apparent and Partial Molar Volumes at Infinite Dilution and Solid–Liquid Equilibria of Dibenzothiophene + Alkane Systems:	https://www.doi.org/10.1021/je200327s
Equilibria of Dibenzothiophene + N-Methyl-2-hydroxyethylammonium Acetate, Butanoate, or Hexanoate Ionic Liquids + Dibenzothiophene + n-Dodecane Systems at 298.2 K and Atmospheric Pressure:	https://www.doi.org/10.1021/je200799u

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132650&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Measurements and prediction of ternary liquid-liquid equilibria for mixtures of IL + sulfur compound + hexadecane:	https://www.doi.org/10.1016/j.fluid.2016.03.014
Thermodynamic analysis for determination of solid - liquid equilibrium of dibenzothiophene in a binary solvent of formic acid and ethanol at different temperatures:	https://www.doi.org/10.1016/j.fluid.2015.08.023
Thermodynamic models for determination of the solubility of dibenzothiophene in pure and binary solvents:	https://www.doi.org/10.1016/j.jct.2014.08.012
Solubility of Dibenzothiophene in Sub- and Supercritical Propane between (278.15 and 333.15) K:	https://www.doi.org/10.1021/je2001667
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Revisiting dibenzothiophene thermochemical data: Experimental and computational studies:	https://www.doi.org/10.1016/j.jct.2009.05.019

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization 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
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