

Dibenzothiophene sulfone

Other names:	1,2,3,4,4a,5a,6,7,8,9,9a,9b-dodecahydrodibenzothiophene 5,5-dioxide Dibenzothiophene S,S-dioxide Dibenzothiophene dioxide Dibenzothiophene, 5,5-dioxide Diphenylene sulfone
Inchi:	InChI=1S/C12H8O2S/c13-15(14)11-7-3-1-5-9(11)10-6-2-4-8-12(10)15/h1-8H
InchiKey:	IKJFYINYNJYDTA-UHFFFAOYSA-N
Formula:	C12H8O2S
SMILES:	O=S1(=O)c2ccccc2-c2ccccc21
Mol. weight [g/mol]:	216.26
CAS:	1016-05-3

Physical Properties

Property code	Value	Unit	Source
gf	-113.42	kJ/mol	Joback Method
hf	-185.39	kJ/mol	Joback Method
hfus	27.17	kJ/mol	Solid-Liquid Equilibria of Dibenzothiophene and Dibenzothiophene Sulfone in Organic Solvents
hvap	65.69	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	9.28	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-4.57		Aqueous Solubility Prediction Method
logp	2.500		Crippen Method
mcvol	149.650	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	566.98	K	Joback Method
tc	800.33	K	Joback Method
tf	419.71	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.75	J/mol×K	566.98	Joback Method
cpg	347.05	J/mol×K	605.87	Joback Method
cpg	359.19	J/mol×K	644.76	Joback Method
cpg	370.26	J/mol×K	683.65	Joback Method
cpg	380.37	J/mol×K	722.55	Joback Method
cpg	389.62	J/mol×K	761.44	Joback Method
cpg	398.12	J/mol×K	800.33	Joback Method
hfust	27.17	kJ/mol	509.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1016053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solid-Liquid Equilibria of Dibenzo[thiophene and Dibenzo[thiophene Sulfone in Organic Solvents:	https://www.doi.org/10.1021/je700234e
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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