

Bis(2-hydroxyphenyl)sulfide

Other names:	Phenol, 2,2'-thiobis- Phenol, 2,2'-thiodi- 2,2'-Dihydroxydiphenyl sulfide 2,2'-Thiodiphenol
Inchi:	InChI=1S/C12H10O2S/c13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)14/h1-8,13-14H
InchiKey:	BLDLRWQLBOJPEB-UHFFFAOYSA-N
Formula:	C12H10O2S
SMILES:	Oc1ccccc1Sc1ccccc1O
Mol. weight [g/mol]:	218.27
CAS:	13693-59-9

Physical Properties

Property code	Value	Unit	Source
gf	-1.14	kJ/mol	Joback Method
hf	-130.70	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	79.70	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	3.249		Crippen Method
mcvol	160.510	ml/mol	McGowan Method
pc	5153.45	kPa	Joback Method
tb	757.34	K	Joback Method
tc	1041.84	K	Joback Method
tf	535.68	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.97	J/molxK	757.34	Joback Method
cpg	429.47	J/molxK	804.76	Joback Method
cpg	440.30	J/molxK	852.17	Joback Method
cpg	450.75	J/molxK	899.59	Joback Method
cpg	461.08	J/molxK	947.01	Joback Method

cpg	471.55	J/mol×K	994.42	Joback Method
cpg	482.43	J/mol×K	1041.84	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13693599&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mconvol:	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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