Bis(phenylthio)methane

Other names:	Bis(phenyithio)methane
	Formaldehyde diphenyl mercaptal
	Bis(thiophenoxy)methane
	Benzene, 1,1'-[methylenebis(thio)]bis-
	[methylenebis(thio)]bisbenzene
Inchi:	InChI=1S/C13H12S2/c1-3-7-12(8-4-1)14-11-15-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	ZHUPZVIALZHGGP-UHFFFAOYSA-N
Formula:	C13H12S2
SMILES:	c1ccc(SCSc2ccccc2)cc1
Mol. weight [g/mol]:	232.36
CAS:	3561-67-9

Physical Properties

Property code	Value	Unit	Source
gf	349.64	kJ/mol	Joback Method
hf	245.15	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.529		Crippen Method
mcvol	179.210	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	687.76	K	Joback Method
tc	970.82	K	Joback Method
tf	357.91	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.79	J/mol×K	687.76	Joback Method
cpg	444.57	J/mol×K	734.94	Joback Method
cpg	458.77	J/mol×K	782.11	Joback Method
cpg	471.45	J/mol×K	829.29	Joback Method

cpg	482.72	J/mol×K	876.47	Joback Method
cpg	492.66	J/mol×K	923.64	Joback Method
cpg	501.35	J/mol×K	970.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C3561679&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvap:	Enthalpy of vaporization at standard conditions
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