

Disulfide, bis(4-methoxyphenyl)

Other names:	Anisole, 4,4'-dithiodi- p-Methoxyphenyl disulfide Bis(p-methoxyphenyl)disulfide Bis(4-methoxyphenyl) disulfide Disulfide, bis(p-methoxyphenyl) 4-Methoxyphenyl disulfide Di(4-methoxyphenyl)disulfide
Inchi:	InChI=1S/C14H14O2S2/c1-15-11-3-7-13(8-4-11)17-18-14-9-5-12(16-2)6-10-14/h3-10H,1
InchiKey:	PZQGLCGLPMWYBT-UHFFFAOYSA-N
Formula:	C14H14O2S2
SMILES:	COc1ccc(SSc2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	278.39
CAS:	5335-87-5

Physical Properties

Property code	Value	Unit	Source
gf	128.80	kJ/mol	Joback Method
hf	-62.87	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
log10ws	-5.00		Crippen Method
logp	4.503		Crippen Method
mvol	205.040	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	765.44	K	Joback Method
tc	1032.04	K	Joback Method
tf	438.68	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.13	J/mol×K	765.44	Joback Method

cpg	542.85	J/mol×K	809.87	Joback Method
cpg	556.05	J/mol×K	854.31	Joback Method
cpg	567.73	J/mol×K	898.74	Joback Method
cpg	577.89	J/mol×K	943.17	Joback Method
cpg	586.52	J/mol×K	987.61	Joback Method
cpg	593.61	J/mol×K	1032.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5335875&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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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