

# Phenyl benzenesulfinyl sulfone

<b>Inchi:</b>	InChI=1S/C12H10O3S2/c13-16(11-7-3-1-4-8-11)17(14,15)12-9-5-2-6-10-12/h1-10H
<b>InchiKey:</b>	GCYFEGKYSQLZAQ-UHFFFAOYSA-N
<b>Formula:</b>	C12H10O3S2
<b>SMILES:</b>	O=S(c1ccccc1)S(=O)(=O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	266.34
<b>CAS:</b>	784-81-6

## Physical Properties

Property code	Value	Unit	Source
gf	-411.27	kJ/mol	Joback Method
hf	-477.04	kJ/mol	Joback Method
hfus	34.05	kJ/mol	Joback Method
hvap	78.22	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.183		Crippen Method
mcvol	182.730	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	633.38	K	Joback Method
tc	875.25	K	Joback Method
tf	352.88	K	Joback Method
vc	0.708	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.45	J/molxK	633.38	Joback Method
cpg	442.75	J/molxK	673.69	Joback Method
cpg	456.68	J/molxK	714.00	Joback Method
cpg	469.26	J/molxK	754.31	Joback Method
cpg	480.52	J/molxK	794.62	Joback Method
cpg	490.50	J/molxK	834.94	Joback Method
cpg	499.21	J/molxK	875.25	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C784816&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C784816&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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