

# Benzonitrile, 4,4'-sulfonyldi

<b>Other names:</b>	4,4'-sulphonylbis(benzonitrile)
<b>Inchi:</b>	InChI=1S/C14H8N2O2S/c15-9-11-1-5-13(6-2-11)19(17,18)14-7-3-12(10-16)4-8-14/h1-8H
<b>InchiKey:</b>	MZKBKRFSDLTYAN-UHFFFAOYSA-N
<b>Formula:</b>	C14H8N2O2S
<b>SMILES:</b>	N#Cc1ccc(S(=O)(=O)c2ccc(C#N)cc2)cc1
<b>Mol. weight [g/mol]:</b>	268.29
<b>CAS:</b>	6461-99-0

## Physical Properties

Property code	Value	Unit	Source
gf	70.38	kJ/mol	Joback Method
hf	-5.76	kJ/mol	Joback Method
hfus	33.71	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.263		Crippen Method
mcvol	191.450	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
tb	834.98	K	Joback Method
tc	1086.64	K	Joback Method
tf	493.96	K	Joback Method
vc	0.781	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.51	J/molxK	834.98	Joback Method
cpg	500.57	J/molxK	876.92	Joback Method
cpg	508.48	J/molxK	918.87	Joback Method
cpg	515.28	J/molxK	960.81	Joback Method
cpg	521.00	J/molxK	1002.75	Joback Method
cpg	525.69	J/molxK	1044.70	Joback Method
cpg	529.37	J/molxK	1086.64	Joback Method

# Sources

<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=C6461990&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6461990&amp;Units=SI</a>
<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>

# 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>mcvol:</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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