

# 4-(4-chlorophenyl)sulfonylaniline

<b>Inchi:</b>	InChI=1S/C12H10ClNO2S/c13-9-1-5-11(6-2-9)17(15,16)12-7-3-10(14)4-8-12/h1-8H,14H
<b>InchiKey:</b>	RWIUBJDOESNTFZ-UHFFFAOYSA-N
<b>Formula:</b>	C12H10ClNO2S
<b>SMILES:</b>	<chem>Nc1ccc(S(=O)(=O)c2ccc(Cl)cc2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	267.74

## Physical Properties

Property code	Value	Unit	Source
gf	-158.30	kJ/mol	Joback Method
hf	-276.19	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	81.84	kJ/mol	Joback Method
log10ws	-4.13		Aqueous Solubility Prediction Method
logp	2.755		Crippen Method
mcvol	182.730	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
tb	695.02	K	Joback Method
tc	944.42	K	Joback Method
tf	454.62	K	Joback Method
vc	0.696	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.80	J/mol×K	695.02	Joback Method
cpg	453.76	J/mol×K	736.59	Joback Method
cpg	465.48	J/mol×K	778.15	Joback Method
cpg	476.01	J/mol×K	819.72	Joback Method
cpg	485.38	J/mol×K	861.29	Joback Method
cpg	493.63	J/mol×K	902.85	Joback Method
cpg	500.80	J/mol×K	944.42	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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