

# 4-amino-N-(4-nitrophenyl)benzenesulfonamide

**Inchi:** InChI=1S/C12H11N3O4S/c13-9-1-7-12(8-2-9)20(18,19)14-10-3-5-11(6-4-10)15(16)17/h1  
**InchiKey:** ACJNABKXDUDYAM-UHFFFAOYSA-N  
**Formula:** C12H11N3O4S  
**SMILES:** Nc1ccc(S(=O)(=O)Nc2ccc([N+](=O)[O-])cc2)cc1  
**Mol. weight [g/mol]:** 293.30

## Physical Properties

Property code	Value	Unit	Source
gf	-21.43	kJ/mol	Joback Method
hf	-217.74	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
hfus	27.90 ± 0.50	kJ/mol	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
hvap	100.48	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	1.978		Crippen Method
mcvol	197.890	ml/mol	McGowan Method
pc	4438.52	kPa	Joback Method
tb	859.60	K	Joback Method
tc	1119.77	K	Joback Method
tf	438.90	K	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
tf	439.00 ± 0.20	K	Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents
vc	0.763	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.24	J/molxK	859.60	Joback Method
cpg	566.19	J/molxK	902.96	Joback Method
cpg	574.78	J/molxK	946.32	Joback Method
cpg	582.06	J/molxK	989.69	Joback Method
cpg	588.10	J/molxK	1033.05	Joback Method
cpg	592.93	J/molxK	1076.41	Joback Method
cpg	596.62	J/molxK	1119.77	Joback Method
psub	4.01e-06	kPa	417.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.18e-06	kPa	409.45	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.30e-06	kPa	412.85	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	3.41e-06	kPa	415.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.50e-06	kPa	405.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	4.34e-06	kPa	418.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	5.46e-06	kPa	420.05	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	5.63e-06	kPa	421.55	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	6.16e-06	kPa	423.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	7.30e-06	kPa	424.65	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	8.92e-06	kPa	426.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.05e-05	kPa	428.75	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.28e-05	kPa	431.35	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

psub	1.41e-05	kPa	432.05	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	1.81e-05	kPa	435.15	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides
psub	2.28e-05	kPa	438.25	Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
Thermodynamic aspects of solubility, solvation and partitioning processes of some sulfonamides:	<a href="https://www.doi.org/10.1016/j.jct.2010.12.007">https://www.doi.org/10.1016/j.jct.2010.12.007</a>
Impact of Sulfonamide Structure on Solubility and Transfer Processes in Biologically Relevant Solvents:	<a href="https://www.doi.org/10.1021/je500918t">https://www.doi.org/10.1021/je500918t</a>
Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<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>psub:</b>	Sublimation 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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