

# Aniline, 4-(n,n-dimethylamino)-2-phenylsulfonyl-

Inchi:	InChI=1S/C14H16N2O2S/c1-16(2)11-8-9-13(15)14(10-11)19(17,18)12-6-4-3-5-7-12/h3-1
InchiKey:	JWRLPQQRYBZAIR-UHFFFAOYSA-N
Formula:	C14H16N2O2S
SMILES:	CN(C)c1ccc(N)c(S(=O)(=O)c2ccccc2)c1
Mol. weight [g/mol]:	276.35
CAS:	19770-80-0

## Physical Properties

Property code	Value	Unit	Source
gf	-18.75	kJ/mol	Joback Method
hf	-234.20	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	83.95	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.168		Crippen Method
mcvol	208.650	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	715.79	K	Joback Method
tc	948.81	K	Joback Method
tf	479.71	K	Joback Method
vc	0.776	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.04	J/molxK	715.79	Joback Method
cpg	573.35	J/molxK	754.63	Joback Method
cpg	587.33	J/molxK	793.46	Joback Method
cpg	600.06	J/molxK	832.30	Joback Method
cpg	611.57	J/molxK	871.14	Joback Method
cpg	621.92	J/molxK	909.98	Joback Method
cpg	631.15	J/molxK	948.81	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=C19770800&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19770800&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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