

# 2-Nitro-4-bromo-benzene-sulfonamide

<b>Inchi:</b>	InChI=1S/C6H5BrN2O4S/c7-4-1-2-6(14(8,12)13)5(3-4)9(10)11/h1-3H,(H2,8,12,13)
<b>InchiKey:</b>	RLOBLCKPLSPZIT-UHFFFAOYSA-N
<b>Formula:</b>	C6H5BrN2O4S
<b>SMILES:</b>	NS(=O)(=O)c1ccc(Br)cc1[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	281.08
<b>CAS:</b>	89581-41-9

## Physical Properties

Property code	Value	Unit	Source
gf	-259.43	kJ/mol	Joback Method
hf	-357.57	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	84.85	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	1.005		Crippen Method
mcvol	144.630	ml/mol	McGowan Method
pc	6944.44	kPa	Joback Method
tb	711.63	K	Joback Method
tc	973.72	K	Joback Method
tf	534.07	K	Joback Method
vc	0.562	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.68	J/molxK	711.63	Joback Method
cpg	334.95	J/molxK	755.31	Joback Method
cpg	342.31	J/molxK	798.99	Joback Method
cpg	348.76	J/molxK	842.67	Joback Method
cpg	354.32	J/molxK	886.35	Joback Method
cpg	359.01	J/molxK	930.03	Joback Method
cpg	362.86	J/molxK	973.72	Joback Method

# Sources

<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=C89581419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C89581419&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>

# 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>hvac:</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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