

# Benzenesulfonamide, n-isobutyl-

<b>Inchi:</b>	InChI=1S/C10H15NO2S/c1-9(2)8-11-14(12,13)10-6-4-3-5-7-10/h3-7,9,11H,8H2,1-2H3
<b>InchiKey:</b>	XRTYMJYAOZHUHI-UHFFFAOYSA-N
<b>Formula:</b>	C10H15NO2S
<b>SMILES:</b>	CC(C)CNS(=O)(=O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	213.30
<b>CAS:</b>	23705-39-7

## Physical Properties

Property code	Value	Unit	Source
gf	-235.86	kJ/mol	Joback Method
hf	-418.36	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.621		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
tb	552.39	K	Joback Method
tc	756.13	K	Joback Method
tf	305.10	K	Joback Method
vc	0.642	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.92	J/molxK	552.39	Joback Method
cpg	402.41	J/molxK	586.35	Joback Method
cpg	416.99	J/molxK	620.30	Joback Method
cpg	430.68	J/molxK	654.26	Joback Method
cpg	443.49	J/molxK	688.22	Joback Method
cpg	455.44	J/molxK	722.18	Joback Method
cpg	466.55	J/molxK	756.13	Joback Method

# Sources

<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>
<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=C23705397&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23705397&amp;Units=SI</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>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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