

# Benzenesulfonamide, 4-methyl-N-ethyl-N-2-ethylhexyl-

<b>Inchi:</b>	InChI=1S/C17H29NO2S/c1-5-8-9-16(6-2)14-18(7-3)21(19,20)17-12-10-15(4)11-13-17/h1
<b>InchiKey:</b>	VJGZWYISHIJAIC-UHFFFAOYSA-N
<b>Formula:</b>	C17H29NO2S
<b>SMILES:</b>	CCCCC(CC)CN(CC)S(=O)(=O)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	311.48

## Physical Properties

Property code	Value	Unit	Source
gf	-165.16	kJ/mol	Joback Method
hf	-560.25	kJ/mol	Joback Method
hfus	44.31	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.222		Crippen Method
mvol	264.700	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	679.80	K	Joback Method
tc	865.66	K	Joback Method
tf	376.32	K	Joback Method
vc	1.018	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.15	J/molxK	679.80	Joback Method
cpg	754.07	J/molxK	710.78	Joback Method
cpg	771.91	J/molxK	741.75	Joback Method
cpg	788.71	J/molxK	772.73	Joback Method
cpg	804.48	J/molxK	803.70	Joback Method
cpg	819.26	J/molxK	834.68	Joback Method
cpg	833.08	J/molxK	865.66	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>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=U415277&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U415277&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<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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