

# N-1-[1,1-bis(p-toluenesulfonylmethyl)propyl]-p-toluenesulfonamide

<b>Inchi:</b>	InChI=1S/C26H31NO8S3/c1-5-26(27-36(28,29)23-12-6-20(2)7-13-23,18-34-37(30,31)24
<b>InchiKey:</b>	HSQMAXWVCAWBHW-UHFFFAOYSA-N
<b>Formula:</b>	C26H31NO8S3
<b>SMILES:</b>	CCC(COS(=O)(=O)c1ccc(C)cc1)(COS(=O)(=O)c1ccc(C)cc1)NS(=O)(=O)c1ccc(C)cc1
<b>Mol. weight [g/mol]:</b>	581.72
<b>CAS:</b>	10405-51-3

## Physical Properties

Property code	Value	Unit	Source
gf	-1047.01	kJ/mol	Joback Method
hf	-1484.56	kJ/mol	Joback Method
hfus	78.25	kJ/mol	Joback Method
hvap	148.15	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	3.850		Crippen Method
mcvol	411.910	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
tb	1124.38	K	Joback Method
tc	1376.62	K	Joback Method
tf	714.82	K	Joback Method
vc	1.605	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.50	J/molxK	1124.38	Joback Method
cpg	1308.77	J/molxK	1166.42	Joback Method
cpg	1309.23	J/molxK	1208.46	Joback Method
cpg	1306.93	J/molxK	1250.50	Joback Method
cpg	1301.90	J/molxK	1292.54	Joback Method
cpg	1294.17	J/molxK	1334.58	Joback Method
cpg	1283.78	J/molxK	1376.62	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=C10405513&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10405513&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>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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