

# Benzenesulfonic acid, 4-methyl-, 1-methylethyl ester

<b>Other names:</b>	isopropyl toluene-4-sulphonate isopropyl p-toluenesulfonate
<b>Inchi:</b>	InChI=1S/C10H14O3S/c1-8(2)13-14(11,12)10-6-4-9(3)5-7-10/h4-8H,1-3H3
<b>InchiKey:</b>	SDQCGKJCBWXRMK-UHFFFAOYSA-N
<b>Formula:</b>	C10H14O3S
<b>SMILES:</b>	<chem>Cc1ccc(S(=O)(=O)OC(C)C)cc1</chem>
<b>Mol. weight [g/mol]:</b>	214.28
<b>CAS:</b>	2307-69-9

## Physical Properties

Property code	Value	Unit	Source
gf	-439.88	kJ/mol	Joback Method
hf	-615.52	kJ/mol	Joback Method
hfus	24.35	kJ/mol	Joback Method
hvap	61.45	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.109		Crippen Method
mvol	161.960	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	529.62	K	Joback Method
tc	731.80	K	Joback Method
tf	287.19	K	Joback Method
vc	0.625	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.85	J/molxK	529.62	Joback Method
cpg	376.78	J/molxK	563.32	Joback Method
cpg	390.95	J/molxK	597.01	Joback Method
cpg	404.38	J/molxK	630.71	Joback Method
cpg	417.06	J/molxK	664.41	Joback Method
cpg	428.99	J/molxK	698.11	Joback Method
cpg	440.17	J/molxK	731.80	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=C2307699&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2307699&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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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