

# 2-Isopropylbenzenethiol, S-methyl-

<b>Inchi:</b>	InChI=1S/C10H14S/c1-8(2)9-6-4-5-7-10(9)11-3/h4-8H,1-3H3
<b>InchiKey:</b>	UWRWHOKKUJISAM-UHFFFAOYSA-N
<b>Formula:</b>	C10H14S
<b>SMILES:</b>	CSc1ccccc1C(C)C
<b>Mol. weight [g/mol]:</b>	166.28

## Physical Properties

Property code	Value	Unit	Source
gf	166.78	kJ/mol	Joback Method
hf	11.92	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	47.22	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.532		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2963.34	kPa	Joback Method
rinsol	1329.00		NIST Webbook
tb	528.20	K	Joback Method
tc	761.14	K	Joback Method
tf	260.80	K	Joback Method
vc	0.535	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.01	J/mol×K	528.20	Joback Method
cpg	325.47	J/mol×K	567.02	Joback Method
cpg	339.98	J/mol×K	605.85	Joback Method
cpg	353.59	J/mol×K	644.67	Joback Method
cpg	366.32	J/mol×K	683.50	Joback Method
cpg	378.20	J/mol×K	722.32	Joback Method
cpg	389.25	J/mol×K	761.14	Joback Method

# Sources

<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>
<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=U353043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U353043&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>rinpol:</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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