

# 2,2'-Thiodi-p-cresol

<b>Inchi:</b>	InChI=1S/C14H14O2S/c1-9-3-5-11(15)13(7-9)17-14-8-10(2)4-6-12(14)16/h3-8,15-16H,1
<b>InchiKey:</b>	CHNWLKJYOVOXOG-UHFFFAOYSA-N
<b>Formula:</b>	C14H14O2S
<b>SMILES:</b>	Cc1ccc(O)c(Sc2cc(C)ccc2O)c1
<b>Mol. weight [g/mol]:</b>	246.32
<b>CAS:</b>	2929-96-6

## Physical Properties

Property code	Value	Unit	Source
gf	-3.56	kJ/mol	Joback Method
hf	-194.92	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	85.48	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.866		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	813.06	K	Joback Method
tc	1084.78	K	Joback Method
tf	583.26	K	Joback Method
vc	0.590	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.68	J/molxK	813.06	Joback Method
cpg	531.62	J/molxK	858.35	Joback Method
cpg	544.06	J/molxK	903.63	Joback Method
cpg	556.23	J/molxK	948.92	Joback Method
cpg	568.34	J/molxK	994.20	Joback Method
cpg	580.62	J/molxK	1039.49	Joback Method
cpg	593.28	J/molxK	1084.78	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=C2929966&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2929966&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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