

# O,o'-sulfinyl dibenzoic acid

<b>Inchi:</b>	InChI=1S/C14H10O5S/c15-13(16)9-5-1-3-7-11(9)20(19)12-8-4-2-6-10(12)14(17)18/h1-8
<b>InchiKey:</b>	HMNPICHEHWVPNJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H10O5S
<b>SMILES:</b>	O=C(O)c1ccccc1S(=O)c1ccccc1C(=O)O
<b>Mol. weight [g/mol]:</b>	290.29
<b>CAS:</b>	52704-04-8

## Physical Properties

Property code	Value	Unit	Source
gf	-476.63	kJ/mol	Joback Method
hf	-617.53	kJ/mol	Joback Method
hfus	38.45	kJ/mol	Joback Method
hvap	112.21	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	2.250		Crippen Method
mcvol	197.700	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	933.42	K	Joback Method
tc	1159.73	K	Joback Method
tf	583.40	K	Joback Method
vc	0.744	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.56	J/molxK	933.42	Joback Method
cpg	557.24	J/molxK	971.14	Joback Method
cpg	563.05	J/molxK	1008.86	Joback Method
cpg	568.01	J/molxK	1046.57	Joback Method
cpg	572.17	J/molxK	1084.29	Joback Method
cpg	575.57	J/molxK	1122.01	Joback Method
cpg	578.23	J/molxK	1159.73	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=C52704048&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52704048&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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