

# Mesurool sulfone

**Other names:**

Phenol, 3,5-dimethyl-4-(methylsulfonyl)-, methylcarbamate  
Carbamic acid, methyl-, 4-(methylsulfonyl)-3,5-xylyl ester  
Ba 51-084786  
Bay 37344 sulfone  
Bayer 37344 Sulfone  
BAY 41790  
Carbamic acid, methyl-, 3,5-dimethyl-4-(methylsulfonyl)phenyl ester  
ENT 25825  
3,5-Xylenol, 4-(methylsulfonyl)-, methylcarbamate  
Methiocarb sulfone

**Inchi:**

InChI=1S/C11H15NO4S/c1-7-5-9(16-11(13)12-3)6-8(2)10(7)17(4,14)15/h5-6H,1-4H3,(H,

**InchiKey:**

RJBJMKAMQIOAML-UHFFFAOYSA-N

**Formula:**

C11H15NO4S

**SMILES:**

CNC(=O)Oc1cc(C)c(S(C)=O)c(C)c1

**Mol. weight [g/mol]:**

257.31

**CAS:**

2179-25-1

## Physical Properties

Property code	Value	Unit	Source
gf	-487.81	kJ/mol	Joback Method
hf	-712.93	kJ/mol	Joback Method
hfus	36.38	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	1.425		Crippen Method
mcvol	187.600	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	666.94	K	Joback Method
tc	871.86	K	Joback Method
tf	441.09	K	Joback Method
vc	0.729	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.63	J/mol×K	666.94	Joback Method
cpg	492.03	J/mol×K	701.09	Joback Method
cpg	504.61	J/mol×K	735.25	Joback Method
cpg	516.35	J/mol×K	769.40	Joback Method
cpg	527.24	J/mol×K	803.56	Joback Method
cpg	537.27	J/mol×K	837.71	Joback Method
cpg	546.43	J/mol×K	871.86	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C2179251&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2179251&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>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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