

# N-Phenethyl O-methyl thiocarbamate

<b>Inchi:</b>	InChI=1S/C10H13NOS/c1-12-10(13)11-8-7-9-5-3-2-4-6-9/h2-6H,7-8H2,1H3,(H,11,13)
<b>InchiKey:</b>	SABSUMPVZBKPRQ-UHFFFAOYSA-N
<b>Formula:</b>	C10H13NOS
<b>SMILES:</b>	COC(S)=NCCc1ccccc1
<b>Mol. weight [g/mol]:</b>	195.28
<b>CAS:</b>	930585-96-9

## Physical Properties

Property code	Value	Unit	Source
hf	-34.51	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.161		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1726.90		NIST Webbook
rinpol	1703.00		NIST Webbook
ripol	2827.00		NIST Webbook
tb	616.72	K	Joback Method
tc	861.88	K	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=C930585969&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C930585969&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvac:</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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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