

# N-Benzyl O-propyl thiocarbamate

<b>Inchi:</b>	InChI=1S/C11H15NOS/c1-2-8-13-11(14)12-9-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3,(H,12,
<b>InchiKey:</b>	KTOIPILWYSRXQY-UHFFFAOYSA-N
<b>Formula:</b>	C11H15NOS
<b>SMILES:</b>	CCCOC(S)=NCc1ccccc1
<b>Mol. weight [g/mol]:</b>	209.31

## Physical Properties

Property code	Value	Unit	Source
hf	-55.15	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.899		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2868.00		NIST Webbook
ripol	2868.00		NIST Webbook
tb	639.60	K	Joback Method
tc	879.51	K	Joback Method

## Sources

<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=R440023&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R440023&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

## 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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