

# 3-(Benzoylamino) thiophane

<b>Inchi:</b>	InChI=1S/C11H13NOS/c13-11(9-4-2-1-3-5-9)12-10-6-7-14-8-10/h1-5,10H,6-8H2,(H,12,1
<b>InchiKey:</b>	DONJDQMILBHKEB-UHFFFAOYSA-N
<b>Formula:</b>	C11H13NOS
<b>SMILES:</b>	OC(=NC1CCSC1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	207.29
<b>CAS:</b>	92367-69-6

## Physical Properties

Property code	Value	Unit	Source
hf	-7.90	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.497		Crippen Method
mcvol	159.130	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
tb	709.61	K	Joback Method
tc	955.15	K	Joback Method

## Sources

<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>
<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=C92367696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C92367696&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation 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

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