

# Butyrimidicthio acid, n-phenyl-, ethyl ester

**Inchi:** InChI=1S/C12H17NS/c1-3-8-12(14-4-2)13-11-9-6-5-7-10-11/h5-7,9-10H,3-4,8H2,1-2H3/t  
**InchiKey:** UWUDNZHWOOEBGE-SEYXRHQNSA-N  
**Formula:** C12H17NS  
**SMILES:** CCCC(=Nc1ccccc1)SCC  
**Mol. weight [g/mol]:** 207.34  
**CAS:** 19255-90-4

## Physical Properties

Property code	Value	Unit	Source
hf	59.82	kJ/mol	Joback Method
hvap	54.79	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.270		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
tb	645.98	K	Joback Method
tc	883.89	K	Joback Method

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C19255904&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** 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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