

# Benzoyl isothiocyanate

<b>Other names:</b>	Benzoic acid, anhydride with isothiocyanic acid Benzoic acid, anhydride with HNCS Benzoylthiocarbimide N-Benzoyl isothiocyanate NSC 29259
<b>Inchi:</b>	InChI=1S/C8H5NOS/c10-8(9-6-11)7-4-2-1-3-5-7/h1-5H
<b>InchiKey:</b>	CPEKAXYCDKETEN-UHFFFAOYSA-N
<b>Formula:</b>	C8H5NOS
<b>SMILES:</b>	O=C(N=C=S)c1ccccc1
<b>Mol. weight [g/mol]:</b>	163.20
<b>CAS:</b>	532-55-8

## Physical Properties

Property code	Value	Unit	Source
hf	199.57	kJ/mol	Joback Method
hvap	52.86	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	1.930		Crippen Method
mcvol	119.120	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	608.94	K	Joback Method
tc	876.34	K	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.00 ± 2.00	K	2.40	NIST Webbook

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

<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=C532558&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C532558&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature

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