

# 3,5-Dimethylphenyl isocyanate

<b>Other names:</b>	3,5-xylol isocyanate Benzene, 1-isocyanato-3,5-dimethyl-
<b>Inchi:</b>	InChI=1S/C9H9NO/c1-7-3-8(2)5-9(4-7)10-6-11/h3-5H,1-2H3
<b>InchiKey:</b>	DZSGDHNHQAJZCO-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO
<b>SMILES:</b>	<chem>Cc1cc(C)cc(N=C=O)c1</chem>
<b>Mol. weight [g/mol]:</b>	147.17
<b>CAS:</b>	54132-75-1

## Physical Properties

Property code	Value	Unit	Source
hf	-20.91	kJ/mol	Joback Method
hvap	48.76	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	2.271		Crippen Method
mvol	121.160	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	508.63	K	Joback Method
tc	728.49	K	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51367e+01
Coeff. B	-4.24003e+03
Coeff. C	-7.73230e+01
Temperature range (K), min.	362.87
Temperature range (K), max.	508.87

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C54132751&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54132751&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>p<sub>vap</sub>:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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