

# Benzene, 1-isocyanato-3-methyl-

<b>Other names:</b>	3-Methylphenyl isocyanate 3-Tolyl isocyanate Isocyanic acid, m-tolyl ester m-Isocyanatotoluene m-Methylphenyl isocyanate m-Tolyl isocyanate
<b>Inchi:</b>	InChI=1S/C8H7NO/c1-7-3-2-4-8(5-7)9-6-10/h2-5H,1H3
<b>InchiKey:</b>	CPPGZWWUPFWALU-UHFFFAOYSA-N
<b>Formula:</b>	C8H7NO
<b>SMILES:</b>	<chem>Cc1cccc(N=C=O)c1</chem>
<b>Mol. weight [g/mol]:</b>	133.15
<b>CAS:</b>	621-29-4

## Physical Properties

Property code	Value	Unit	Source
hf	11.20	kJ/mol	Joback Method
hvap	45.87	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
log10ws	-6.43		Crippen Method
logp	1.962		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	480.77	K	Joback Method
tc	703.01	K	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	8.99653e+00
Coeff. B	-1.84267e+03
Coeff. C	-3.79360e+01

Temperature range (K), min.	249.52
Temperature range (K), max.	537.98

## Sources

<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/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C621294&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C621294&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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