

# Hexane, 1-isocyanato-

<b>Other names:</b>	1-hexyl isocyanate Hexyl isocyanate n-Hexyl isocyanate
<b>Inchi:</b>	InChI=1S/C7H13NO/c1-2-3-4-5-6-8-7-9/h2-6H2,1H3
<b>InchiKey:</b>	ANJPRQPHZGHVQB-UHFFFAOYSA-N
<b>Formula:</b>	C7H13NO
<b>SMILES:</b>	CCCCCN=C=O
<b>Mol. weight [g/mol]:</b>	127.18
<b>CAS:</b>	2525-62-4

## Physical Properties

Property code	Value	Unit	Source
hf	-193.22	kJ/mol	Joback Method
hvap	40.71	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	1.903		Crippen Method
mvol	116.740	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	426.23	K	Joback Method
tc	602.94	K	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.45763e+01
Coeff. B	-3.85111e+03
Coeff. C	-6.24000e+01
Temperature range (K), min.	331.92
Temperature range (K), max.	478.07

# Sources

<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=C2525624&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2525624&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/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>

# 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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