

# 2,4,6-Trimethylphenyl isocyanide

<b>Inchi:</b>	InChI=1S/C10H11N/c1-7-5-8(2)10(11-4)9(3)6-7/h5-6H,1-3H3
<b>InchiKey:</b>	PNLRXQFLTHXBIT-UHFFFAOYSA-N
<b>Formula:</b>	C10H11N
<b>SMILES:</b>	[C-]#[N+]c1c(C)cc(C)cc1C
<b>Mol. weight [g/mol]:</b>	145.20
<b>CAS:</b>	57116-96-8

## Physical Properties

Property code	Value	Unit	Source
chs	-5608.20 ± 4.70	kJ/mol	NIST Webbook
gf	250.02	kJ/mol	Joback Method
hf	167.50 ± 4.90	kJ/mol	NIST Webbook
hfs	101.00 ± 4.70	kJ/mol	NIST Webbook
hfus	16.04	kJ/mol	Joback Method
hsub	66.40 ± 1.50	kJ/mol	NIST Webbook
hsub	66.50	kJ/mol	NIST Webbook
hvap	52.59	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.163		Crippen Method
mcvol	129.380	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	571.90	K	Joback Method
tc	798.39	K	Joback Method
tf	331.43	K	Joback Method
vc	0.513	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.16	J/mol×K	571.90	Joback Method
cpg	297.82	J/mol×K	609.65	Joback Method
cpg	308.84	J/mol×K	647.40	Joback Method
cpg	319.24	J/mol×K	685.14	Joback Method
cpg	329.03	J/mol×K	722.89	Joback Method

cpg	338.24	J/mol×K	760.64	Joback Method
cpg	346.88	J/mol×K	798.39	Joback Method
cps	241.80	J/mol×K	298.15	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57116968&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57116968&amp;Units=SI</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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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