

# O-toluidine, n-isopropyl-

<b>Inchi:</b>	InChI=1S/C10H15N/c1-8(2)11-10-7-5-4-6-9(10)3/h4-8,11H,1-3H3
<b>InchiKey:</b>	NKVWOHIEVZXVGP-UHFFFAOYSA-N
<b>Formula:</b>	C10H15N
<b>SMILES:</b>	Cc1ccccc1NC(C)C
<b>Mol. weight [g/mol]:</b>	149.23
<b>CAS:</b>	2100-43-8

## Physical Properties

Property code	Value	Unit	Source
gf	223.05	kJ/mol	Joback Method
hf	23.52	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	46.84	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.815		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	2950.48	kPa	Joback Method
tb	509.59	K	Joback Method
tc	721.82	K	Joback Method
tf	279.06	K	Joback Method
vc	0.516	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.12	J/mol×K	509.59	Joback Method
cpg	320.37	J/mol×K	544.96	Joback Method
cpg	334.75	J/mol×K	580.33	Joback Method
cpg	348.31	J/mol×K	615.70	Joback Method
cpg	361.08	J/mol×K	651.07	Joback Method
cpg	373.08	J/mol×K	686.44	Joback Method
cpg	384.35	J/mol×K	721.82	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2100438&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2100438&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>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion 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>mccvol:</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

Latest version available from:

<https://www.chemeo.com/cid/76-412-0/O-toluidine-n-isopropyl.pdf>

Generated by Cheméo on 2024-04-20 14:05:52.395247483 +0000 UTC m=+15911201.315824795.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.