

# 2-Chloro-5-nitrobenzyl alcohol, isopropyl ether

<b>Inchi:</b>	InChI=1S/C10H12ClNO3/c1-7(2)15-6-8-5-9(12(13)14)3-4-10(8)11/h3-5,7H,6H2,1-2H3
<b>InchiKey:</b>	DTHLKNLMHFEEKGM-UHFFFAOYSA-N
<b>Formula:</b>	C10H12ClNO3
<b>SMILES:</b>	CC(C)OCc1cc([N+](=O)[O-])ccc1Cl
<b>Mol. weight [g/mol]:</b>	229.66

## Physical Properties

Property code	Value	Unit	Source
gf	42.65	kJ/mol	Joback Method
hf	-200.14	kJ/mol	Joback Method
hfus	28.14	kJ/mol	Joback Method
hvap	64.45	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.173		Crippen Method
mcvol	163.530	ml/mol	McGowan Method
pc	2738.28	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	676.09	K	Joback Method
tc	915.95	K	Joback Method
tf	434.68	K	Joback Method
vc	0.630	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.78	J/mol×K	676.09	Joback Method
cpg	418.54	J/mol×K	716.07	Joback Method
cpg	430.39	J/mol×K	756.04	Joback Method
cpg	441.35	J/mol×K	796.02	Joback Method
cpg	451.43	J/mol×K	836.00	Joback Method
cpg	460.67	J/mol×K	875.98	Joback Method
cpg	469.08	J/mol×K	915.95	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U378152&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378152&amp;Units=SI</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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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