

# 2-Chloro-5-nitrobenzyl alcohol, n-propyl ether

<b>Inchi:</b>	InChI=1S/C10H12ClNO3/c1-2-5-15-7-8-6-9(12(13)14)3-4-10(8)11/h3-4,6H,2,5,7H2,1H3
<b>InchiKey:</b>	VTQSLSRSEDIMHD-UHFFFAOYSA-N
<b>Formula:</b>	C10H12ClNO3
<b>SMILES:</b>	CCCOc1cc([N+](=O)[O-])ccc1Cl
<b>Mol. weight [g/mol]:</b>	229.66

## Physical Properties

Property code	Value	Unit	Source
gf	45.09	kJ/mol	Joback Method
hf	-194.86	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.175		Crippen Method
mvol	163.530	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	676.53	K	Joback Method
tc	911.56	K	Joback Method
tf	449.68	K	Joback Method
vc	0.636	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.22	J/mol×K	676.53	Joback Method
cpg	417.70	J/mol×K	715.70	Joback Method
cpg	429.31	J/mol×K	754.87	Joback Method
cpg	440.08	J/mol×K	794.04	Joback Method
cpg	450.02	J/mol×K	833.22	Joback Method
cpg	459.16	J/mol×K	872.39	Joback Method
cpg	467.52	J/mol×K	911.56	Joback Method

# 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=U378153&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378153&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

# 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>h vap:</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>r in pol:</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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