

# 2,3-Dichlorobenzyl alcohol, tert.-butyl ether

<b>Inchi:</b>	InChI=1S/C11H14Cl2O/c1-11(2,3)14-7-8-5-4-6-9(12)10(8)13/h4-6H,7H2,1-3H3
<b>InchiKey:</b>	FYAFCBBJJQFART-UHFFFAOYSA-N
<b>Formula:</b>	C11H14Cl2O
<b>SMILES:</b>	CC(C)(C)OCc1cccc(Cl)c1Cl
<b>Mol. weight [g/mol]:</b>	233.13

## Physical Properties

Property code	Value	Unit	Source
gf	8.87	kJ/mol	Joback Method
hf	-229.23	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.308		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinsol	1540.00		NIST Webbook
tb	581.77	K	Joback Method
tc	806.74	K	Joback Method
tf	349.68	K	Joback Method
vc	0.648	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.44	J/molxK	581.77	Joback Method
cpg	399.68	J/molxK	619.26	Joback Method
cpg	412.99	J/molxK	656.76	Joback Method
cpg	425.41	J/molxK	694.25	Joback Method
cpg	436.98	J/molxK	731.75	Joback Method
cpg	447.75	J/molxK	769.24	Joback Method
cpg	457.75	J/molxK	806.74	Joback Method
dvisc	0.0014821	Paxs	349.68	Joback Method
dvisc	0.0008427	Paxs	388.36	Joback Method

dvisc	0.0005307	Paxs	427.04	Joback Method
dvisc	0.0003609	Paxs	465.73	Joback Method
dvisc	0.0002604	Paxs	504.41	Joback Method
dvisc	0.0001968	Paxs	543.09	Joback Method
dvisc	0.0001544	Paxs	581.77	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375303&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375303&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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