

# 2,4,6-Trichlorobenzyl alcohol, isopropyl ether

<b>Inchi:</b>	InChI=1S/C10H11Cl3O/c1-6(2)14-5-8-9(12)3-7(11)4-10(8)13/h3-4,6H,5H2,1-2H3
<b>InchiKey:</b>	NXEXDEPKKPGTBC-UHFFFAOYSA-N
<b>Formula:</b>	C10H11Cl3O
<b>SMILES:</b>	CC(C)OCc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	253.55

## Physical Properties

Property code	Value	Unit	Source
gf	-26.39	kJ/mol	Joback Method
hf	-232.33	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.572		Crippen Method
mcvol	170.590	ml/mol	McGowan Method
pc	2470.27	kPa	Joback Method
rinpol	1564.00		NIST Webbook
tb	604.09	K	Joback Method
tc	829.18	K	Joback Method
tf	363.43	K	Joback Method
vc	0.646	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.56	J/molxK	604.09	Joback Method
cpg	412.12	J/molxK	791.67	Joback Method
cpg	402.95	J/molxK	754.15	Joback Method
cpg	393.12	J/molxK	716.64	Joback Method
cpg	382.62	J/molxK	679.12	Joback Method
cpg	371.44	J/molxK	641.61	Joback Method
cpg	420.64	J/molxK	829.18	Joback Method
dvisc	0.0001647	Paxs	604.09	Joback Method
dvisc	0.0002037	Paxs	563.98	Joback Method

dvisc	0.0002603	Paxs	523.87	Joback Method
dvisc	0.0003463	Paxs	483.76	Joback Method
dvisc	0.0004853	Paxs	443.65	Joback Method
dvisc	0.0007273	Paxs	403.54	Joback Method
dvisc	0.0011917	Paxs	363.43	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375278&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375278&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>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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