

# Benzyl alcohol, «alpha», «alpha»-dimethyl-p-isopropyl-

<b>Other names:</b>	Benzenemethanol, «alpha», «alpha»-dimethyl-4-(1-methylethyl)- «alpha», «alpha»-Dimethyl-p-isopropylbenzyl alcohol p-Hydroxydiisopropylbenzene p-Oxidiisopropylbenzene 2-(4-Isopropylphenyl)-2-propanol
<b>Inchi:</b>	InChI=1S/C12H18O/c1-9(2)10-5-7-11(8-6-10)12(3,4)13/h5-9,13H,1-4H3
<b>InchiKey:</b>	VBSMBCNJC BKQFP-UHFFFAOYSA-N
<b>Formula:</b>	C12H18O
<b>SMILES:</b>	CC(C)c1ccc(C(C)(C)O)cc1
<b>Mol. weight [g/mol]:</b>	178.27
<b>CAS:</b>	3445-42-9

## Physical Properties

Property code	Value	Unit	Source
chs	-6950.90 ± 2.80	kJ/mol	NIST Webbook
gf	16.52	kJ/mol	Joback Method
hf	-232.21	kJ/mol	Joback Method
hfs	-343.70 ± 2.80	kJ/mol	NIST Webbook
hfus	13.64	kJ/mol	Joback Method
hvap	60.24	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.037		Crippen Method
mvol	162.050	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	594.13	K	Joback Method
tc	797.22	K	Joback Method
tf	312.18	K	Joback Method
vc	0.602	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.79	J/mol×K	797.22	Joback Method
cpg	410.21	J/mol×K	594.13	Joback Method

cpg	424.92	J/mol×K	627.98	Joback Method
cpg	438.71	J/mol×K	661.83	Joback Method
cpg	451.64	J/mol×K	695.68	Joback Method
cpg	463.77	J/mol×K	729.52	Joback Method
cpg	475.14	J/mol×K	763.37	Joback Method
dvisc	0.0000622	Paxs	594.13	Joback Method
dvisc	0.0112775	Paxs	312.18	Joback Method
dvisc	0.0026894	Paxs	359.17	Joback Method
dvisc	0.0008936	Paxs	406.16	Joback Method
dvisc	0.0003731	Paxs	453.15	Joback Method
dvisc	0.0001836	Paxs	500.15	Joback Method
dvisc	0.0001020	Paxs	547.14	Joback Method
hsubt	100.80 ± 1.80	kJ/mol	302.00	NIST Webbook

## 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=C3445429&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3445429&amp;Units=SI</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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