

# 2,3,6-Trifluorobenzyl alcohol, 1-methylpropyl ether

Inchi:	InChI=1S/C11H13F3O/c1-3-7(2)15-6-8-9(12)4-5-10(13)11(8)14/h4-5,7H,3,6H2,1-2H3
InchiKey:	UENRBYMKSQQLCB-UHFFFAOYSA-N
Formula:	C11H13F3O
SMILES:	CCC(C)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]:	218.22

## Physical Properties

Property code	Value	Unit	Source
gf	-566.61	kJ/mol	Joback Method
hf	-794.08	kJ/mol	Joback Method
hfus	24.03	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.419		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinsol	1197.00		NIST Webbook
tb	512.49	K	Joback Method
tc	692.17	K	Joback Method
tf	286.71	K	Joback Method
vc	0.610	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.76	J/mol×K	512.49	Joback Method
cpg	364.68	J/mol×K	542.44	Joback Method
cpg	377.06	J/mol×K	572.38	Joback Method
cpg	388.92	J/mol×K	602.33	Joback Method
cpg	400.27	J/mol×K	632.28	Joback Method
cpg	411.10	J/mol×K	662.22	Joback Method
cpg	421.43	J/mol×K	692.17	Joback Method

# Sources

<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=U375265&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375265&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>

# 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>hvac:</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>mccol:</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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