

# 2,3,6-Trifluorobenzyl alcohol, n-propyl ether

<b>Inchi:</b>	InChI=1S/C10H11F3O/c1-2-5-14-6-7-8(11)3-4-9(12)10(7)13/h3-4H,2,5-6H2,1H3
<b>InchiKey:</b>	TZKPPELOOIVYGT-UHFFFAOYSA-N
<b>Formula:</b>	C10H11F3O
<b>SMILES:</b>	CCCOc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	204.19

## Physical Properties

Property code	Value	Unit	Source
gf	-572.59	kJ/mol	Joback Method
hf	-768.16	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	42.08	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.030		Crippen Method
mcvol	139.180	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinsol	1151.00		NIST Webbook
tb	490.05	K	Joback Method
tc	667.77	K	Joback Method
tf	290.44	K	Joback Method
vc	0.559	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.37	J/mol×K	490.05	Joback Method
cpg	319.01	J/mol×K	519.67	Joback Method
cpg	330.20	J/mol×K	549.29	Joback Method
cpg	340.95	J/mol×K	578.91	Joback Method
cpg	351.25	J/mol×K	608.53	Joback Method
cpg	361.12	J/mol×K	638.15	Joback Method
cpg	370.54	J/mol×K	667.77	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U375267&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375267&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>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>rinpola:</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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