

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

<b>Inchi:</b>	InChI=1S/C11H13F3O/c1-2-3-6-15-7-8-9(12)4-5-10(13)11(8)14/h4-5H,2-3,6-7H2,1H3
<b>InchiKey:</b>	LRVYVEFFMRRREF-UHFFFAOYSA-N
<b>Formula:</b>	C11H13F3O
<b>SMILES:</b>	CCCCOCc1c(F)ccc(F)c1F
<b>Mol. weight [g/mol]:</b>	218.22

## Physical Properties

Property code	Value	Unit	Source
gf	-564.17	kJ/mol	Joback Method
hf	-788.80	kJ/mol	Joback Method
hfus	27.55	kJ/mol	Joback Method
hvap	44.30	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.421		Crippen Method
mcvol	153.270	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1247.00		NIST Webbook
rinpol	1247.00		NIST Webbook
tb	512.93	K	Joback Method
tc	689.06	K	Joback Method
tf	301.71	K	Joback Method
vc	0.616	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.51	J/molxK	512.93	Joback Method
cpg	364.10	J/molxK	542.28	Joback Method
cpg	376.20	J/molxK	571.64	Joback Method
cpg	387.79	J/molxK	600.99	Joback Method
cpg	398.90	J/molxK	630.35	Joback Method
cpg	409.52	J/molxK	659.70	Joback Method
cpg	419.67	J/molxK	689.06	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=U375266&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375266&amp;Units=SI</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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