

# 2-Chloro-6-fluorobenzyl alcohol, isopropyl ether

Inchi:	InChI=1S/C10H12ClFO/c1-7(2)13-6-8-9(11)4-3-5-10(8)12/h3-5,7H,6H2,1-2H3
InchiKey:	LCAGIUAMUFTSHZ-UHFFFAOYSA-N
Formula:	C10H12ClFO
SMILES:	CC(C)OCc1c(F)cccc1Cl
Mol. weight [g/mol]:	202.65

## Physical Properties

Property code	Value	Unit	Source
gf	-187.71	kJ/mol	Joback Method
hf	-385.49	kJ/mol	Joback Method
hfus	19.86	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.404		Crippen Method
mcvol	147.880	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinsol	1264.00		NIST Webbook
tb	523.52	K	Joback Method
tc	728.35	K	Joback Method
tf	291.66	K	Joback Method
vc	0.567	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.00	J/mol×K	523.52	Joback Method
cpg	330.99	J/mol×K	557.66	Joback Method
cpg	343.33	J/mol×K	591.80	Joback Method
cpg	355.05	J/mol×K	625.94	Joback Method
cpg	366.14	J/mol×K	660.07	Joback Method
cpg	376.62	J/mol×K	694.21	Joback Method
cpg	386.51	J/mol×K	728.35	Joback Method

# Sources

<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=U378144&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U378144&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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