

# 2-Chloro-5-nitrobenzyl alcohol, chlorodifluoroacetate

<b>Inchi:</b>	InChI=1S/C9H5Cl2F2NO4/c10-7-2-1-6(14(16)17)3-5(7)4-18-8(15)9(11,12)13/h1-3H,4H2
<b>InchiKey:</b>	WFHXBRUFNWLXHP-UHFFFAOYSA-N
<b>Formula:</b>	C9H5Cl2F2NO4
<b>SMILES:</b>	O=C(OCc1cc([N+](=O)[O-])ccc1Cl)C(F)(F)Cl
<b>Mol. weight [g/mol]:</b>	300.04

## Physical Properties

Property code	Value	Unit	Source
gf	-490.96	kJ/mol	Joback Method
hf	-703.51	kJ/mol	Joback Method
hfus	33.62	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.123		Crippen Method
mcvol	166.790	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	740.26	K	Joback Method
tc	979.89	K	Joback Method
tf	521.86	K	Joback Method
vc	0.660	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.13	J/molxK	740.26	Joback Method
cpg	412.45	J/molxK	780.20	Joback Method
cpg	419.95	J/molxK	820.14	Joback Method
cpg	426.69	J/molxK	860.08	Joback Method
cpg	432.70	J/molxK	900.01	Joback Method
cpg	438.05	J/molxK	939.95	Joback Method
cpg	442.78	J/molxK	979.89	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U376109&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376109&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>hvp:</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>rinp:</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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