

# 2,3-Dichlorobenzyl alcohol, chlorodifluoroacetate

Inchi:	InChI=1S/C9H5Cl3F2O2/c10-6-3-1-2-5(7(6)11)4-16-8(15)9(12,13)14/h1-3H,4H2
InchiKey:	JKQHABOISPOZFR-UHFFFAOYSA-N
Formula:	C9H5Cl3F2O2
SMILES:	O=C(OCc1cccc(Cl)c1Cl)C(F)(F)Cl
Mol. weight [g/mol]:	289.49

## Physical Properties

Property code	Value	Unit	Source
gf	-538.44	kJ/mol	Joback Method
hf	-708.49	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.868		Crippen Method
mcvol	161.610	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	625.85	K	Joback Method
tc	848.15	K	Joback Method
tf	408.17	K	Joback Method
vc	0.627	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.89	J/mol×K	625.85	Joback Method
cpg	353.90	J/mol×K	662.90	Joback Method
cpg	362.19	J/mol×K	699.95	Joback Method
cpg	369.78	J/mol×K	737.00	Joback Method
cpg	376.72	J/mol×K	774.05	Joback Method
cpg	383.04	J/mol×K	811.10	Joback Method
cpg	388.78	J/mol×K	848.15	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=U376079&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376079&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>

# 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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