

# Benzene, 1-chloro-3-chlorofluoromethyl

<b>Inchi:</b>	InChI=1S/C7H5Cl2F/c8-6-3-1-2-5(4-6)7(9)10/h1-4,7H
<b>InchiKey:</b>	OXPZSMIDBFQBNW-UHFFFAOYSA-N
<b>Formula:</b>	C7H5Cl2F
<b>SMILES:</b>	FC(Cl)c1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	179.02

## Physical Properties

Property code	Value	Unit	Source
gf	-110.27	kJ/mol	Joback Method
hf	-195.62	kJ/mol	Joback Method
hfus	15.49	kJ/mol	Joback Method
hvap	41.68	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.547		Crippen Method
mvol	111.980	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1126.00		NIST Webbook
tb	464.91	K	Joback Method
tc	685.73	K	Joback Method
tf	253.02	K	Joback Method
vc	0.429	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.41	J/mol×K	464.91	Joback Method
cpg	204.98	J/mol×K	501.71	Joback Method
cpg	213.90	J/mol×K	538.52	Joback Method
cpg	222.22	J/mol×K	575.32	Joback Method
cpg	229.94	J/mol×K	612.13	Joback Method
cpg	237.11	J/mol×K	648.93	Joback Method
cpg	243.76	J/mol×K	685.73	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=R515078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R515078&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>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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