

# Crotyl alcohol, trifluoroacetate

<b>Inchi:</b>	InChI=1S/C6H7F3O2/c1-2-3-4-11-5(10)6(7,8)9/h2-3H,4H2,1H3/b3-2+
<b>InchiKey:</b>	XBSBZMNVXMVAHP-NSCUHMNNSA-N
<b>Formula:</b>	C6H7F3O2
<b>SMILES:</b>	CC=CCOC(=O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	168.11

## Physical Properties

Property code	Value	Unit	Source
gf	-735.65	kJ/mol	Joback Method
hf	-891.83	kJ/mol	Joback Method
hfus	16.11	kJ/mol	Joback Method
hvap	34.32	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.668		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinsol	737.60		NIST Webbook
tb	411.71	K	Joback Method
tc	580.99	K	Joback Method
tf	228.65	K	Joback Method
vc	0.418	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.48	J/mol×K	411.71	Joback Method
cpg	220.77	J/mol×K	439.92	Joback Method
cpg	229.57	J/mol×K	468.14	Joback Method
cpg	237.91	J/mol×K	496.35	Joback Method
cpg	245.80	J/mol×K	524.57	Joback Method
cpg	253.26	J/mol×K	552.78	Joback Method
cpg	260.31	J/mol×K	580.99	Joback Method

# Sources

<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>
<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=U352266&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352266&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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