

# 4-(Trifluoromethyl)benzoic acid, 3-chloroprop-2-enyl ester

<b>Inchi:</b>	InChI=1S/C11H8ClF3O2/c12-6-1-7-17-10(16)8-2-4-9(5-3-8)11(13,14)15/h1-6H,7H2/b6-1
<b>InchiKey:</b>	WAVIARCGALFILB-LZCJLJQNSA-N
<b>Formula:</b>	C11H8ClF3O2
<b>SMILES:</b>	O=C(OCC=CCl)c1ccc(C(F)(F)F)cc1
<b>Mol. weight [g/mol]:</b>	264.63

## Physical Properties

Property code	Value	Unit	Source
gf	-602.70	kJ/mol	Joback Method
hf	-785.71	kJ/mol	Joback Method
hfus	26.91	kJ/mol	Joback Method
hvap	52.77	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.615		Crippen Method
mcvol	162.780	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1434.00		NIST Webbook
rinpol	1434.00		NIST Webbook
tb	595.20	K	Joback Method
tc	800.74	K	Joback Method
tf	353.86	K	Joback Method
vc	0.639	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.52	J/mol×K	595.20	Joback Method
cpg	391.98	J/mol×K	629.46	Joback Method
cpg	402.62	J/mol×K	663.71	Joback Method
cpg	412.48	J/mol×K	697.97	Joback Method
cpg	421.60	J/mol×K	732.23	Joback Method
cpg	430.04	J/mol×K	766.48	Joback Method
cpg	437.85	J/mol×K	800.74	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=U299448&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299448&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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