

# 4-Fluoro-3-(trifluoromethyl)benzoyl chloride

<b>Other names:</b>	Benzoyl chloride, 4-fluoro-3-(trifluoromethyl)-
<b>Inchi:</b>	InChI=1S/C8H3ClF4O/c9-7(14)4-1-2-6(10)5(3-4)8(11,12)13/h1-3H
<b>InchiKey:</b>	BUDISZQHCHGLJW-UHFFFAOYSA-N
<b>Formula:</b>	C8H3ClF4O
<b>SMILES:</b>	O=C(Cl)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	226.56
<b>CAS:</b>	67515-56-4

## Physical Properties

Property code	Value	Unit	Source
gf	-807.62	kJ/mol	Joback Method
hf	-916.37	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	43.57	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.224		Crippen Method
mcvol	120.710	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
tb	504.23	K	Joback Method
tc	702.93	K	Joback Method
tf	316.01	K	Joback Method
vc	0.491	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.84	J/mol×K	504.23	Joback Method
cpg	261.87	J/mol×K	537.35	Joback Method
cpg	270.24	J/mol×K	570.46	Joback Method
cpg	277.99	J/mol×K	603.58	Joback Method
cpg	285.15	J/mol×K	636.69	Joback Method
cpg	291.75	J/mol×K	669.81	Joback Method
cpg	297.83	J/mol×K	702.93	Joback Method

# Sources

<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=C67515564&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C67515564&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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