

# Benzene, 1-ethoxy-3-fluoro-

<b>Other names:</b>	Phenetole, m-fluoro-
<b>Inchi:</b>	InChI=1S/C8H9FO/c1-2-10-8-5-3-4-7(9)6-8/h3-6H,2H2,1H3
<b>InchiKey:</b>	UWWCZZMOTBWUAB-UHFFFAOYSA-N
<b>Formula:</b>	C8H9FO
<b>SMILES:</b>	CCOc1cccc(F)c1
<b>Mol. weight [g/mol]:</b>	140.15
<b>CAS:</b>	458-03-7

## Physical Properties

Property code	Value	Unit	Source
chl	-4269.40	kJ/mol	NIST Webbook
gf	-180.55	kJ/mol	Joback Method
hf	-311.72	kJ/mol	Joback Method
hfus	14.40	kJ/mol	Joback Method
hvap	37.93	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	2.224		Crippen Method
mcvol	107.460	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	435.79	K	Joback Method
tc	634.28	K	Joback Method
tf	241.68	K	Joback Method
vc	0.411	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.33	J/molxK	435.79	Joback Method
cpg	218.63	J/molxK	468.87	Joback Method
cpg	229.42	J/molxK	501.95	Joback Method
cpg	239.72	J/molxK	535.04	Joback Method
cpg	249.52	J/molxK	568.12	Joback Method
cpg	258.84	J/molxK	601.20	Joback Method
cpg	267.69	J/molxK	634.28	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.40	K	2.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>KDB:</b>	<a href="https://www.cheric.org/files/research/kdb/mol/mol1808.mol">https://www.cheric.org/files/research/kdb/mol/mol1808.mol</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=C458037&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C458037&amp;Units=SI</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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