

# Allyl fluoride

<b>Other names:</b>	1-Fluoro-2-propene 1-Propene, 3-fluoro- 3-Fluoro-1-propene 3-Fluoropropene 3-Fluoropropylene CH <sub>2</sub> =CHCH <sub>2</sub> F Propene, 3-fluoro-
<b>Inchi:</b>	InChI=1S/C3H5F/c1-2-3-4/h2H,1,3H2
<b>InchiKey:</b>	QCMKXHXKNIQBBC-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>3</sub> H <sub>5</sub> F
<b>SMILES:</b>	C=CCF
<b>Mol. weight [g/mol]:</b>	60.07
<b>CAS:</b>	818-92-8

## Physical Properties

Property code	Value	Unit	Source
gf	-132.59	kJ/mol	Joback Method
hf	-175.93	kJ/mol	Joback Method
hfus	5.33	kJ/mol	Joback Method
hvap	20.79	kJ/mol	Joback Method
ie	10.56	eV	NIST Webbook
ie	10.38	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
log10ws	-0.79		Crippen Method
logp	1.142		Crippen Method
mvol	50.600	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
rinpol	380.00		NIST Webbook
tb	263.00	K	NIST Webbook
tc	416.81	K	Joback Method
tf	122.40	K	Joback Method
vc	0.203	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	65.76	J/molxK	263.99	Joback Method
cpg	70.66	J/molxK	289.46	Joback Method
cpg	75.39	J/molxK	314.93	Joback Method
cpg	79.94	J/molxK	340.40	Joback Method
cpg	84.33	J/molxK	365.87	Joback Method
cpg	88.55	J/molxK	391.34	Joback Method
cpg	92.61	J/molxK	416.81	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.66321e+01
Coeff. B	-2.96437e+03
Coeff. C	-1.62520e+01
Temperature range (K), min.	197.62
Temperature range (K), max.	287.51

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C818928&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C818928&amp;Units=SI</a>
The Yaws Handbook of Vapor Pressure:	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<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>ie:</b>	Ionization energy
<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>pvap:</b>	Vapor 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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