

# (4-Fluorophenyl) methanol, 3-methylbutyl ether

Inchi:	InChI=1S/C12H17FO/c1-10(2)7-8-14-9-11-3-5-12(13)6-4-11/h3-6,10H,7-9H2,1-2H3
InchiKey:	AECPCNPICIXGIQ-UHFFFAOYSA-N
Formula:	C12H17FO
SMILES:	CC(C)CCOCc1ccc(F)cc1
Mol. weight [g/mol]:	196.26

## Physical Properties

Property code	Value	Unit	Source
gf	-149.31	kJ/mol	Joback Method
hf	-399.56	kJ/mol	Joback Method
hfus	21.23	kJ/mol	Joback Method
hvap	46.45	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.388		Crippen Method
mvol	163.820	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
tb	526.87	K	Joback Method
tc	720.16	K	Joback Method
tf	271.76	K	Joback Method
vc	0.629	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.83	J/mol×K	526.87	Joback Method
cpg	396.55	J/mol×K	559.09	Joback Method
cpg	411.52	J/mol×K	591.30	Joback Method
cpg	425.75	J/mol×K	623.52	Joback Method
cpg	439.26	J/mol×K	655.73	Joback Method
cpg	452.06	J/mol×K	687.95	Joback Method
cpg	464.18	J/mol×K	720.16	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=U374666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374666&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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