

# Fumaric acid, 3-methylbutyl 2-fluorophenyl ester

Inchi:	InChI=1S/C15H17FO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-6-4-3-5-12(13)16/h3-8,11
InchiKey:	RNYJOXILEFWWII-BQYQJAHWSA-N
Formula:	C15H17FO4
SMILES:	CC(C)CCOC(=O)C=CC(=O)Oc1ccccc1F
Mol. weight [g/mol]:	280.29

## Physical Properties

Property code	Value	Unit	Source
gf	-406.67	kJ/mol	Joback Method
hf	-701.64	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.877		Crippen Method
mcvol	210.800	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1897.00		NIST Webbook
rinpol	1897.00		NIST Webbook
tb	729.83	K	Joback Method
tc	935.84	K	Joback Method
tf	422.58	K	Joback Method
vc	0.807	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.05	J/mol×K	729.83	Joback Method
cpg	591.92	J/mol×K	764.17	Joback Method
cpg	604.88	J/mol×K	798.50	Joback Method
cpg	616.95	J/mol×K	832.84	Joback Method
cpg	628.15	J/mol×K	867.17	Joback Method
cpg	638.50	J/mol×K	901.51	Joback Method
cpg	648.02	J/mol×K	935.84	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405550&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405550&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvp:</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>rinp:</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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