

# Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 3-fluorophenyl ester

InChI: 1S/C17H13ClFNO4/c1-23-15-6-5-11(18)9-14(15)20-16(21)7-8-17(22)24-13-4-2-3-  
InChIKey: OUPHRINUOIQUNI-BQYQJAHWSA-N

Formula: C17H13ClFNO4

SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 349.74

## Physical Properties

Property code	Value	Unit	Source
gf	-216.78	kJ/mol	Joback Method
hf	-486.32	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.588		Crippen Method
mcvol	237.440	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinqol	3037.00		NIST Webbook
tb	900.27	K	Joback Method
tc	1134.70	K	Joback Method
tf	594.16	K	Joback Method
vc	0.901	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.76	J/molxK	900.27	Joback Method
cpg	673.05	J/molxK	939.34	Joback Method
cpg	682.26	J/molxK	978.41	Joback Method
cpg	690.42	J/molxK	1017.49	Joback Method
cpg	697.57	J/molxK	1056.56	Joback Method
cpg	703.76	J/molxK	1095.63	Joback Method
cpg	709.02	J/molxK	1134.70	Joback Method

# Sources

<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>
<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=U357490&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357490&amp;Units=SI</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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