

# o-Methoxybenzoic acid, 5-fluoro-2-nitrophenyl ester

Inchi:	InChI=1S/C14H10FNO5/c1-20-12-5-3-2-4-10(12)14(17)21-13-8-9(15)6-7-11(13)16(18)19
InchiKey:	KGEYFHFHBKZIDE-UHFFFAOYSA-N
Formula:	C14H10FNO5
SMILES:	COc1ccccc1C(=O)Oc1cc(F)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	291.23

## Physical Properties

Property code	Value	Unit	Source
gf	-235.25	kJ/mol	Joback Method
hf	-477.53	kJ/mol	Joback Method
hfus	37.35	kJ/mol	Joback Method
hvap	80.64	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	2.962		Crippen Method
mcvol	193.100	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinqol	2020.10		NIST Webbook
tb	837.84	K	Joback Method
tc	1086.14	K	Joback Method
tf	576.53	K	Joback Method
vc	0.746	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.22	J/molxK	837.84	Joback Method
cpg	550.03	J/molxK	879.22	Joback Method
cpg	559.64	J/molxK	920.61	Joback Method
cpg	568.05	J/molxK	961.99	Joback Method
cpg	575.30	J/molxK	1003.37	Joback Method
cpg	581.39	J/molxK	1044.75	Joback Method
cpg	586.33	J/molxK	1086.14	Joback Method

# Sources

<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=U292620&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292620&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>
<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>

# 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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