

# 2-Fluoro-3-trifluoromethylbenzoic acid, 4-nitrophenyl ester

<b>Inchi:</b>	InChI=1S/C14H7F4NO4/c15-12-10(2-1-3-11(12)14(16,17)18)13(20)23-9-6-4-8(5-7-9)19(
<b>InchiKey:</b>	ORVWIWVUMDEEPF-UHFFFAOYSA-N
<b>Formula:</b>	C14H7F4NO4
<b>SMILES:</b>	O=C(Oc1ccc([N+](=O)[O-])cc1)c1cccc(C(F)(F)F)c1F
<b>Mol. weight [g/mol]:</b>	329.20

## Physical Properties

Property code	Value	Unit	Source
gf	-711.84	kJ/mol	Joback Method
hf	-942.39	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	3.972		Crippen Method
mcvol	192.540	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	810.00	K	Joback Method
tc	1044.90	K	Joback Method
tf	558.49	K	Joback Method
vc	0.770	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.75	J/mol×K	810.00	Joback Method
cpg	549.60	J/mol×K	849.15	Joback Method
cpg	558.47	J/mol×K	888.30	Joback Method
cpg	566.42	J/mol×K	927.45	Joback Method
cpg	573.51	J/mol×K	966.60	Joback Method
cpg	579.81	J/mol×K	1005.75	Joback Method
cpg	585.39	J/mol×K	1044.90	Joback Method

# Sources

<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=U357653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357653&amp;Units=SI</a>
<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>

# 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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