

# 4-Fluoro-2-trifluoromethylbenzoic acid, hexyl ester

Inchi:	InChI=1S/C14H16F4O2/c1-2-3-4-5-8-20-13(19)11-7-6-10(15)9-12(11)14(16,17)18/h6-7,9
InchiKey:	ZLOCAAUTTZCELM-UHFFFAOYSA-N
Formula:	C14H16F4O2
SMILES:	CCCCCCOC(=O)c1ccc(F)cc1C(F)(F)F
Mol. weight [g/mol]:	292.27

## Physical Properties

Property code	Value	Unit	Source
gf	-850.17	kJ/mol	Joback Method
hf	-1156.69	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	54.95	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.582		Crippen Method
mcvol	198.880	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
tb	626.50	K	Joback Method
tc	806.72	K	Joback Method
tf	375.94	K	Joback Method
vc	0.796	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.75	J/mol×K	626.50	Joback Method
cpg	542.70	J/mol×K	656.54	Joback Method
cpg	555.89	J/mol×K	686.57	Joback Method
cpg	568.33	J/mol×K	716.61	Joback Method
cpg	580.06	J/mol×K	746.64	Joback Method
cpg	591.11	J/mol×K	776.68	Joback Method
cpg	601.49	J/mol×K	806.72	Joback Method

# Sources

<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.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=U338823&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338823&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>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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