

# 6-Fluoro-2-trifluoromethylbenzoic acid, propyl ester

Inchi:	InChI=1S/C11H10F4O2/c1-2-6-17-10(16)9-7(11(13,14)15)4-3-5-8(9)12/h3-5H,2,6H2,1H3
InchiKey:	NMMKHVCNVYPESR-UHFFFAOYSA-N
Formula:	C11H10F4O2
SMILES:	CCCOC(=O)c1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]:	250.19

## Physical Properties

Property code	Value	Unit	Source
gf	-875.43	kJ/mol	Joback Method
hf	-1094.77	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	48.27	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.411		Crippen Method
mvol	156.610	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
rinpol	1241.00		NIST Webbook
rinpol	1241.00		NIST Webbook
tb	557.86	K	Joback Method
tc	743.16	K	Joback Method
tf	342.13	K	Joback Method
vc	0.628	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.19	J/molxK	557.86	Joback Method
cpg	394.31	J/molxK	588.74	Joback Method
cpg	405.75	J/molxK	619.63	Joback Method
cpg	416.53	J/molxK	650.51	Joback Method
cpg	426.68	J/molxK	681.40	Joback Method
cpg	436.21	J/molxK	712.28	Joback Method
cpg	445.15	J/molxK	743.16	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=U338976&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338976&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.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>

# 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>h vap:</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>r in pol:</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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