

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

<b>Inchi:</b>	InChI=1S/C13H14F4O2/c1-12(2,3)7-19-11(18)10-8(13(15,16)17)5-4-6-9(10)14/h4-6H,7H
<b>InchiKey:</b>	LLXOHOIKMAKRCS-UHFFFAOYSA-N
<b>Formula:</b>	C13H14F4O2
<b>SMILES:</b>	CC(C)(C)COC(=O)c1c(F)cccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	278.24

## Physical Properties

Property code	Value	Unit	Source
gf	-855.75	kJ/mol	Joback Method
hf	-1144.80	kJ/mol	Joback Method
hfus	22.97	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.047		Crippen Method
mcvol	184.790	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
rinsol	1307.00		NIST Webbook
tb	600.39	K	Joback Method
tc	791.41	K	Joback Method
tf	367.09	K	Joback Method
vc	0.730	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.60	J/mol×K	600.39	Joback Method
cpg	495.65	J/mol×K	632.23	Joback Method
cpg	508.79	J/mol×K	664.06	Joback Method
cpg	521.09	J/mol×K	695.90	Joback Method
cpg	532.59	J/mol×K	727.74	Joback Method
cpg	543.32	J/mol×K	759.58	Joback Method
cpg	553.33	J/mol×K	791.41	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=U357690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357690&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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