

# 5-Fluoro-3-trifluoromethylbenzoic acid, octyl ester

<b>Inchi:</b>	InChI=1S/C16H20F4O2/c1-2-3-4-5-6-7-8-22-15(21)12-9-13(16(18,19)20)11-14(17)10-12
<b>InchiKey:</b>	OHBLVCJNANQISF-UHFFFAOYSA-N
<b>Formula:</b>	C16H20F4O2
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cc(F)cc(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	320.32

## Physical Properties

Property code	Value	Unit	Source
gf	-833.33	kJ/mol	Joback Method
hf	-1197.97	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	59.40	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.362		Crippen Method
mcvol	227.060	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	1651.00		NIST Webbook
rinpol	1651.00		NIST Webbook
tb	672.26	K	Joback Method
tc	850.60	K	Joback Method
tf	398.48	K	Joback Method
vc	0.908	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.67	J/mol×K	672.26	Joback Method
cpg	648.54	J/mol×K	701.98	Joback Method
cpg	662.59	J/mol×K	731.71	Joback Method
cpg	675.86	J/mol×K	761.43	Joback Method
cpg	688.38	J/mol×K	791.15	Joback Method
cpg	700.16	J/mol×K	820.88	Joback Method
cpg	711.25	J/mol×K	850.60	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=U338900&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338900&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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