

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

Inchi:	InChI=1S/C20H28F4O2/c1-3-5-6-7-8-9-10-11-18(4-2)26-19(25)15-12-16(20(22,23)24)14
InchiKey:	GKQBAPMHLFQMSI-UHFFFAOYSA-N
Formula:	C20H28F4O2
SMILES:	CCCCCCCCC(CC)OC(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]:	376.43

## Physical Properties

Property code	Value	Unit	Source
gf	-802.09	kJ/mol	Joback Method
hf	-1285.81	kJ/mol	Joback Method
hfus	44.99	kJ/mol	Joback Method
hvap	67.92	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.921		Crippen Method
mcvol	283.420	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	763.34	K	Joback Method
tc	944.85	K	Joback Method
tf	428.56	K	Joback Method
vc	1.127	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.25	J/mol×K	763.34	Joback Method
cpg	874.80	J/mol×K	793.59	Joback Method
cpg	890.39	J/mol×K	823.84	Joback Method
cpg	905.08	J/mol×K	854.10	Joback Method
cpg	918.89	J/mol×K	884.35	Joback Method
cpg	931.87	J/mol×K	914.60	Joback Method
cpg	944.06	J/mol×K	944.85	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338656&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338656&amp;Units=SI</a>
<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>

# 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>hvp:</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>rinp:</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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