

# 3-Methoxy-2,4,5-trifluorobenzoic acid, dodecyl ester

<b>Inchi:</b>	InChI=1S/C20H29F3O3/c1-3-4-5-6-7-8-9-10-11-12-13-26-20(24)15-14-16(21)18(23)19(2
<b>InchiKey:</b>	ZIFLUPHYNIDULO-UHFFFAOYSA-N
<b>Formula:</b>	C20H29F3O3
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)c1cc(F)c(F)c(OC)c1F
<b>Mol. weight [g/mol]:</b>	374.44

## Physical Properties

Property code	Value	Unit	Source
gf	-731.94	kJ/mol	Joback Method
hf	-1230.83	kJ/mol	Joback Method
hfus	53.26	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.190		Crippen Method
mvol	287.520	ml/mol	McGowan Method
pc	1131.38	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	800.12	K	Joback Method
tc	984.17	K	Joback Method
tf	487.82	K	Joback Method
vc	1.143	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.22	J/mol×K	800.12	Joback Method
cpg	894.55	J/mol×K	830.80	Joback Method
cpg	909.93	J/mol×K	861.47	Joback Method
cpg	924.36	J/mol×K	892.15	Joback Method
cpg	937.85	J/mol×K	922.82	Joback Method
cpg	950.41	J/mol×K	953.50	Joback Method
cpg	962.05	J/mol×K	984.17	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338769&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338769&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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