

# 5-Fluoro-2-trifluoromethylbenzoic acid, dodecyl ester

Inchi:	InChI=1S/C20H28F4O2/c1-2-3-4-5-6-7-8-9-10-11-14-26-19(25)17-15-16(21)12-13-18(17)
InchiKey:	MZYIUHKUTAPUTO-UHFFFAOYSA-N
Formula:	C20H28F4O2
SMILES:	CCCCCCCCCCCCOC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	376.43

## Physical Properties

Property code	Value	Unit	Source
gf	-799.65	kJ/mol	Joback Method
hf	-1280.53	kJ/mol	Joback Method
hfus	48.51	kJ/mol	Joback Method
hvap	68.31	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.922		Crippen Method
mcvol	283.420	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	763.78	K	Joback Method
tc	943.85	K	Joback Method
tf	443.56	K	Joback Method
vc	1.133	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.75	J/mol×K	763.78	Joback Method
cpg	874.15	J/mol×K	793.79	Joback Method
cpg	889.63	J/mol×K	823.80	Joback Method
cpg	904.22	J/mol×K	853.81	Joback Method
cpg	917.96	J/mol×K	883.82	Joback Method
cpg	930.88	J/mol×K	913.84	Joback Method
cpg	943.03	J/mol×K	943.85	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=U338748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338748&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.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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