

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

Inchi:	InChI=1S/C25H38F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-31-24(30)22-20-21
InchiKey:	MRBKCOPQGSLDCS-UHFFFAOYSA-N
Formula:	C25H38F4O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cc(F)ccc1C(F)(F)F
Mol. weight [g/mol]:	446.56

## Physical Properties

Property code	Value	Unit	Source
gf	-757.55	kJ/mol	Joback Method
hf	-1383.73	kJ/mol	Joback Method
hfus	61.46	kJ/mol	Joback Method
hvap	79.44	kJ/mol	Joback Method
log10ws	-9.85		Crippen Method
logp	8.873		Crippen Method
mcvol	353.870	ml/mol	McGowan Method
pc	849.00	kPa	Joback Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
tb	878.18	K	Joback Method
tc	1075.21	K	Joback Method
tf	499.91	K	Joback Method
vc	1.413	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.56	J/mol×K	878.18	Joback Method
cpg	1177.13	J/mol×K	911.02	Joback Method
cpg	1194.54	J/mol×K	943.86	Joback Method
cpg	1210.84	J/mol×K	976.70	Joback Method
cpg	1226.09	J/mol×K	1009.53	Joback Method
cpg	1240.36	J/mol×K	1042.37	Joback Method
cpg	1253.72	J/mol×K	1075.21	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U338753&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338753&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>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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