

# 2-Fluoro-3-trifluoromethylbenzoic acid, hexadecyl ester

<b>Inchi:</b>	InChI=1S/C24H36F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-30-23(29)20-17-16-18
<b>InchiKey:</b>	JYUDIGHCKGWSLR-UHFFFAOYSA-N
<b>Formula:</b>	C24H36F4O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C(F)(F)F)c1F
<b>Mol. weight [g/mol]:</b>	432.54

## Physical Properties

Property code	Value	Unit	Source
gf	-765.97	kJ/mol	Joback Method
hf	-1363.09	kJ/mol	Joback Method
hfus	58.87	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-9.43		Crippen Method
logp	8.483		Crippen Method
mvol	339.780	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	855.30	K	Joback Method
tc	1047.30	K	Joback Method
tf	488.64	K	Joback Method
vc	1.357	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.90	J/molxK	855.30	Joback Method
cpg	1114.97	J/molxK	887.30	Joback Method
cpg	1131.93	J/molxK	919.30	Joback Method
cpg	1147.85	J/molxK	951.30	Joback Method
cpg	1162.76	J/molxK	983.30	Joback Method
cpg	1176.74	J/molxK	1015.30	Joback Method
cpg	1189.84	J/molxK	1047.30	Joback Method

# Sources

<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=U338731&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338731&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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