

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

Inchi:	InChI=1S/C18H24F4O2/c1-2-3-4-5-6-7-8-9-13-24-17(23)14-11-10-12-15(16(14)19)18(20)
InchiKey:	QIZAYTUOHNNKKKE-UHFFFAOYSA-N
Formula:	C18H24F4O2
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]:	348.38

## Physical Properties

Property code	Value	Unit	Source
gf	-816.49	kJ/mol	Joback Method
hf	-1239.25	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	6.142		Crippen Method
mcvol	255.240	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
tb	718.02	K	Joback Method
tc	896.17	K	Joback Method
tf	421.02	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.55	J/mol×K	718.02	Joback Method
cpg	759.20	J/mol×K	747.71	Joback Method
cpg	774.00	J/mol×K	777.40	Joback Method
cpg	787.96	J/mol×K	807.10	Joback Method
cpg	801.12	J/mol×K	836.79	Joback Method
cpg	813.51	J/mol×K	866.48	Joback Method
cpg	825.17	J/mol×K	896.17	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=U338725&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338725&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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