

# 3-Trifluoromethylbenzoic acid, undec-2-enyl ester

Inchi:	InChI=1S/C19H25F3O2/c1-2-3-4-5-6-7-8-9-10-14-24-18(23)16-12-11-13-17(15-16)19(20)
InchiKey:	AAZFDMMASBCQRR-MDZDMXLPSA-N
Formula:	C19H25F3O2
SMILES:	CCCCCCCCC=CCOC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	342.40

## Physical Properties

Property code	Value	Unit	Source
gf	-523.41	kJ/mol	Joback Method
hf	-935.09	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.169		Crippen Method
mvol	263.260	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2008.00		NIST Webbook
rinpol	2008.00		NIST Webbook
tb	740.81	K	Joback Method
tc	927.72	K	Joback Method
tf	414.10	K	Joback Method
vc	1.038	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.01	J/molxK	740.81	Joback Method
cpg	785.09	J/molxK	771.96	Joback Method
cpg	800.23	J/molxK	803.11	Joback Method
cpg	814.49	J/molxK	834.27	Joback Method
cpg	827.91	J/molxK	865.42	Joback Method
cpg	840.56	J/molxK	896.57	Joback Method
cpg	852.47	J/molxK	927.72	Joback Method

# Sources

<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=U299327&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299327&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpolar:</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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