

# 4-Fluoro-3-trifluoromethylbenzoic acid, eicosyl ester

<b>Inchi:</b>	InChI=1S/C28H44F4O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-34-27(33)
<b>InchiKey:</b>	BQLDLKXIQFNBL-LUHFFFAOYSA-N
<b>Formula:</b>	C28H44F4O2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCOC(=O)c1ccc(F)c(C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	488.64

## Physical Properties

Property code	Value	Unit	Source
gf	-732.29	kJ/mol	Joback Method
hf	-1445.65	kJ/mol	Joback Method
hfus	69.23	kJ/mol	Joback Method
hvap	86.11	kJ/mol	Joback Method
log10ws	-11.10		Crippen Method
logp	10.043		Crippen Method
mvol	396.140	ml/mol	McGowan Method
pc	722.63	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	946.82	K	Joback Method
tc	1165.03	K	Joback Method
tf	533.72	K	Joback Method
vc	1.581	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.17	J/mol×K	946.82	Joback Method
cpg	1367.59	J/mol×K	983.19	Joback Method
cpg	1386.59	J/mol×K	1019.56	Joback Method
cpg	1404.26	J/mol×K	1055.93	Joback Method
cpg	1420.71	J/mol×K	1092.30	Joback Method
cpg	1436.02	J/mol×K	1128.66	Joback Method
cpg	1450.30	J/mol×K	1165.03	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.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=U338932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338932&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>hvpap:</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>rinppl:</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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