

# trans-3-(Trifluoromethyl)cinnamic acid, octadecyl ester

Inchi:	InChI=1S/C28H43F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-33-27(32)22-21
InchiKey:	BFSFHQUZLDFAY-QURGRASLSA-N
Formula:	C28H43F3O2
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C=Cc1ccc(C(F)(F)F)c1
Mol. weight [g/mol]:	468.63

## Physical Properties

Property code	Value	Unit	Source
gf	-447.63	kJ/mol	Joback Method
hf	-1120.85	kJ/mol	Joback Method
hfus	66.74	kJ/mol	Joback Method
hvap	86.23	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	9.523		Crippen Method
mcvol	390.070	ml/mol	McGowan Method
pc	768.19	kPa	Joback Method
rinsol	3060.00		NIST Webbook
tb	946.73	K	Joback Method
tc	1160.79	K	Joback Method
tf	515.53	K	Joback Method
vc	1.542	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1312.74	J/mol×K	946.73	Joback Method
cpg	1332.59	J/mol×K	982.41	Joback Method
cpg	1351.23	J/mol×K	1018.08	Joback Method
cpg	1368.78	J/mol×K	1053.76	Joback Method
cpg	1385.33	J/mol×K	1089.44	Joback Method
cpg	1400.99	J/mol×K	1125.12	Joback Method
cpg	1415.87	J/mol×K	1160.79	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=U299879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299879&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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