

# trans-3-Trifluoromethylcinnamic acid, tridec-2-ynyl ester

Inchi:	InChI=1S/C23H29F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-18-28-22(27)17-16-20-14-13-15-21
InchiKey:	PEJDJMJWTWLNBE-WUKNDPDISA-N
Formula:	C23H29F3O2
SMILES:	CCCCCCCCC#CCOC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	394.47

## Physical Properties

Property code	Value	Unit	Source
gf	-286.93	kJ/mol	Joback Method
hf	-745.35	kJ/mol	Joback Method
hfus	56.91	kJ/mol	Joback Method
hvap	77.25	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.796		Crippen Method
mcvol	311.020	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2665.00		NIST Webbook
tb	841.33	K	Joback Method
tc	1041.14	K	Joback Method
tf	565.28	K	Joback Method
vc	1.224	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.22	J/molxK	841.33	Joback Method
cpg	968.80	J/molxK	874.63	Joback Method
cpg	984.39	J/molxK	907.93	Joback Method
cpg	999.04	J/molxK	941.24	Joback Method
cpg	1012.84	J/molxK	974.54	Joback Method
cpg	1025.85	J/molxK	1007.84	Joback Method
cpg	1038.13	J/molxK	1041.14	Joback Method

# Sources

<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=U299419&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299419&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.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>

# 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>h vap:</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>m cvol:</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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