

# 2,5-Di(trifluoromethyl)benzoic acid, tridecyl ester

Inchi:	InChI=1S/C22H30F6O2/c1-2-3-4-5-6-7-8-9-10-11-12-15-30-20(29)18-16-17(21(23,24)25
InchiKey:	HHPDXYAESUCGCY-UHFFFAOYSA-N
Formula:	C22H30F6O2
SMILES:	CCCCCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	440.46

## Physical Properties

Property code	Value	Unit	Source
gf	-1169.59	kJ/mol	Joback Method
hf	-1722.78	kJ/mol	Joback Method
hfus	52.44	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.192		Crippen Method
mvol	315.140	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	804.85	K	Joback Method
tc	987.23	K	Joback Method
tf	469.70	K	Joback Method
vc	1.270	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.74	J/molxK	804.85	Joback Method
cpg	1008.32	J/molxK	835.25	Joback Method
cpg	1023.92	J/molxK	865.64	Joback Method
cpg	1038.60	J/molxK	896.04	Joback Method
cpg	1052.41	J/molxK	926.44	Joback Method
cpg	1065.41	J/molxK	956.83	Joback Method
cpg	1077.67	J/molxK	987.23	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=U338946&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338946&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>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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