

# 2,5-Di(trifluoromethyl)benzoic acid, 3-pentadecyl ester

**Inchi:** InChI=1S/C24H34F6O2/c1-3-5-6-7-8-9-10-11-12-13-14-19(4-2)32-22(31)20-17-18(23(25  
**InchiKey:** NQIWYOHSFVHIRN-UHFFFAOYSA-N  
**Formula:** C24H34F6O2  
**SMILES:** CCCCCCCCCCCC(CC)OC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F  
**Mol. weight [g/mol]:** 468.52

## Physical Properties

Property code	Value	Unit	Source
gf	-1155.19	kJ/mol	Joback Method
hf	-1769.34	kJ/mol	Joback Method
hfus	54.09	kJ/mol	Joback Method
hvap	73.89	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	8.971		Crippen Method
mcvol	343.320	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
tb	850.17	K	Joback Method
tc	1040.95	K	Joback Method
tf	477.24	K	Joback Method
vc	1.375	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1112.53	J/molxK	850.17	Joback Method
cpg	1130.07	J/molxK	881.97	Joback Method
cpg	1146.54	J/molxK	913.76	Joback Method
cpg	1162.00	J/molxK	945.56	Joback Method
cpg	1176.52	J/molxK	977.35	Joback Method
cpg	1190.16	J/molxK	1009.15	Joback Method
cpg	1203.02	J/molxK	1040.95	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=U338710&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338710&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>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>rlnol:</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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