

# 3,4-Difluorobenzoic acid, pentadecyl ester

<b>Inchi:</b>	InChI=1S/C22H34F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-26-22(25)19-15-16-20(23)
<b>InchiKey:</b>	DOZMTPZUTLUQQI-UHFFFAOYSA-N
<b>Formula:</b>	C22H34F2O2
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	368.50

## Physical Properties

Property code	Value	Unit	Source
gf	-396.03	kJ/mol	Joback Method
hf	-920.84	kJ/mol	Joback Method
hfus	54.95	kJ/mol	Joback Method
hvap	75.69	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.213		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
pc	1058.95	kPa	Joback Method
rinpol	2474.00		NIST Webbook
rinpol	2474.00		NIST Webbook
tb	814.23	K	Joback Method
tc	1001.16	K	Joback Method
tf	462.50	K	Joback Method
vc	1.220	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.82	J/molxK	814.23	Joback Method
cpg	977.64	J/molxK	845.38	Joback Method
cpg	994.43	J/molxK	876.54	Joback Method
cpg	1010.21	J/molxK	907.69	Joback Method
cpg	1025.02	J/molxK	938.85	Joback Method
cpg	1038.89	J/molxK	970.00	Joback Method
cpg	1051.85	J/molxK	1001.16	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=U338871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338871&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>hvap:</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>rinpolar:</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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