

# 3,4-Difluorobenzoic acid, 6-pentadecyl ester

<b>Inchi:</b>	InChI=1S/C22H34F2O2/c1-3-5-7-8-9-10-12-14-19(13-11-6-4-2)26-22(25)18-15-16-20(23
<b>InchiKey:</b>	AFXPOXGAUXQONN-UHFFFAOYSA-N
<b>Formula:</b>	C22H34F2O2
<b>SMILES:</b>	CCCCCCCCC(CCCCC)OC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	368.50

## Physical Properties

Property code	Value	Unit	Source
gf	-398.47	kJ/mol	Joback Method
hf	-926.12	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	75.30	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.211		Crippen Method
mcvol	308.060	ml/mol	McGowan Method
pc	1064.48	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	813.79	K	Joback Method
tc	1001.75	K	Joback Method
tf	447.50	K	Joback Method
vc	1.214	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.31	J/mol×K	813.79	Joback Method
cpg	978.23	J/mol×K	845.12	Joback Method
cpg	995.09	J/mol×K	876.44	Joback Method
cpg	1010.93	J/mol×K	907.77	Joback Method
cpg	1025.77	J/mol×K	939.09	Joback Method
cpg	1039.66	J/mol×K	970.42	Joback Method
cpg	1052.62	J/mol×K	1001.75	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<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=U338615&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338615&amp;Units=SI</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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