

# 3,4-Difluorobenzoic acid, 5-tetradecyl ester

**Inchi:** InChI=1S/C21H32F2O2/c1-3-5-7-8-9-10-11-13-18(12-6-4-2)25-21(24)17-14-15-19(22)20  
**InchiKey:** HBWHTCYWKGEBEEA-UHFFFAOYSA-N  
**Formula:** C21H32F2O2  
**SMILES:** CCCCCCCCCC(CCCC)OC(=O)c1ccc(F)c(F)c1  
**Mol. weight [g/mol]:** 354.47

## Physical Properties

Property code	Value	Unit	Source
gf	-406.89	kJ/mol	Joback Method
hf	-905.48	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	6.821		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1134.43	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	790.91	K	Joback Method
tc	977.04	K	Joback Method
tf	436.23	K	Joback Method
vc	1.157	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.46	J/mol×K	790.91	Joback Method
cpg	918.04	J/mol×K	821.93	Joback Method
cpg	934.61	J/mol×K	852.95	Joback Method
cpg	950.21	J/mol×K	883.98	Joback Method
cpg	964.85	J/mol×K	915.00	Joback Method
cpg	978.57	J/mol×K	946.02	Joback Method
cpg	991.40	J/mol×K	977.04	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=U338608&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338608&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>rinpola:</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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