

# 3,4-Difluorobenzoic acid, hexyl ester

<b>Inchi:</b>	InChI=1S/C13H16F2O2/c1-2-3-4-5-8-17-13(16)10-6-7-11(14)12(15)9-10/h6-7,9H,2-5,8H
<b>InchiKey:</b>	PAEJZHBPMRUCT-UHFFFAOYSA-N
<b>Formula:</b>	C13H16F2O2
<b>SMILES:</b>	CCCCCCOC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	242.26

## Physical Properties

Property code	Value	Unit	Source
gf	-471.81	kJ/mol	Joback Method
hf	-735.08	kJ/mol	Joback Method
hfus	31.64	kJ/mol	Joback Method
hvap	55.65	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.702		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpola	1549.00		NIST Webbook
rinpola	1549.00		NIST Webbook
tb	608.31	K	Joback Method
tc	796.03	K	Joback Method
tf	361.07	K	Joback Method
vc	0.716	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.91	J/molxK	608.31	Joback Method
cpg	472.91	J/molxK	639.60	Joback Method
cpg	486.22	J/molxK	670.88	Joback Method
cpg	498.84	J/molxK	702.17	Joback Method
cpg	510.79	J/molxK	733.46	Joback Method
cpg	522.08	J/molxK	764.74	Joback Method
cpg	532.72	J/molxK	796.03	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338862&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338862&amp;Units=SI</a>
<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>hvpap:</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>rinpól:</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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