

# 3,4-Difluorobenzoic acid, heptyl ester

**Inchi:** InChI=1S/C14H18F2O2/c1-2-3-4-5-6-9-18-14(17)11-7-8-12(15)13(16)10-11/h7-8,10H,2-6  
**InchiKey:** COGOHGGQSAAJTR-UHFFFAOYSA-N  
**Formula:** C14H18F2O2  
**SMILES:** CCCCCCOC(=O)c1ccc(F)c(F)c1  
**Mol. weight [g/mol]:** 256.29

## Physical Properties

Property code	Value	Unit	Source
gf	-463.39	kJ/mol	Joback Method
hf	-755.72	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	57.88	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.092		Crippen Method
mvol	195.340	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	631.19	K	Joback Method
tc	817.08	K	Joback Method
tf	372.34	K	Joback Method
vc	0.771	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.59	J/mol×K	631.19	Joback Method
cpg	524.18	J/mol×K	662.17	Joback Method
cpg	538.04	J/mol×K	693.15	Joback Method
cpg	551.17	J/mol×K	724.13	Joback Method
cpg	563.60	J/mol×K	755.12	Joback Method
cpg	575.34	J/mol×K	786.10	Joback Method
cpg	586.41	J/mol×K	817.08	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=U338863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338863&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>h vap:</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>r in pol:</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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