

# 3,4-Difluorobenzoic acid, decyl ester

<b>Inchi:</b>	InChI=1S/C17H24F2O2/c1-2-3-4-5-6-7-8-9-12-21-17(20)14-10-11-15(18)16(19)13-14/h1
<b>InchiKey:</b>	BQPUIPCCEZZAU-UHFFFAOYSA-N
<b>Formula:</b>	C17H24F2O2
<b>SMILES:</b>	CCCCCCCCCOC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	298.37

## Physical Properties

Property code	Value	Unit	Source
gf	-438.13	kJ/mol	Joback Method
hf	-817.64	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.262		Crippen Method
mvol	237.610	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	699.83	K	Joback Method
tc	882.34	K	Joback Method
tf	406.15	K	Joback Method
vc	0.940	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.96	J/mol×K	699.83	Joback Method
cpg	685.95	J/mol×K	730.25	Joback Method
cpg	701.10	J/mol×K	760.67	Joback Method
cpg	715.44	J/mol×K	791.09	Joback Method
cpg	728.99	J/mol×K	821.50	Joback Method
cpg	741.75	J/mol×K	851.92	Joback Method
cpg	753.76	J/mol×K	882.34	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=U338866&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338866&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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