

# 3,4-Difluorobenzoic acid, 4-dodecyl ester

<b>Inchi:</b>	InChI=1S/C19H28F2O2/c1-3-5-6-7-8-9-11-16(10-4-2)23-19(22)15-12-13-17(20)18(21)14
<b>InchiKey:</b>	WBIUDEYXKUJGNB-UHFFFAOYSA-N
<b>Formula:</b>	C19H28F2O2
<b>SMILES:</b>	CCCCCCCCC(CCC)OC(=O)c1ccc(F)c(F)c1
<b>Mol. weight [g/mol]:</b>	326.42

## Physical Properties

Property code	Value	Unit	Source
gf	-423.73	kJ/mol	Joback Method
hf	-864.20	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.041		Crippen Method
mvol	265.790	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	745.15	K	Joback Method
tc	929.57	K	Joback Method
tf	413.69	K	Joback Method
vc	1.046	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.42	J/mol×K	745.15	Joback Method
cpg	800.35	J/mol×K	775.89	Joback Method
cpg	816.35	J/mol×K	806.62	Joback Method
cpg	831.44	J/mol×K	837.36	Joback Method
cpg	845.65	J/mol×K	868.10	Joback Method
cpg	859.00	J/mol×K	898.84	Joback Method
cpg	871.51	J/mol×K	929.57	Joback Method

# Sources

<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=U338597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338597&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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