

# 2,5-Difluorobenzoic acid, 3-tridecyl ester

<b>Inchi:</b>	InChI=1S/C20H30F2O2/c1-3-5-6-7-8-9-10-11-12-17(4-2)24-20(23)18-15-16(21)13-14-19
<b>InchiKey:</b>	AGBFKNUSQQIFNE-UHFFFAOYSA-N
<b>Formula:</b>	C20H30F2O2
<b>SMILES:</b>	CCCCCCCCCCC(CC)OC(=O)c1cc(F)ccc1F
<b>Mol. weight [g/mol]:</b>	340.45

## Physical Properties

Property code	Value	Unit	Source
gf	-415.31	kJ/mol	Joback Method
hf	-884.84	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	70.85	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.431		Crippen Method
mvol	279.880	ml/mol	McGowan Method
pc	1211.51	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	768.03	K	Joback Method
tc	953.00	K	Joback Method
tf	424.96	K	Joback Method
vc	1.101	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.47	J/mol×K	768.03	Joback Method
cpg	858.73	J/mol×K	798.86	Joback Method
cpg	875.02	J/mol×K	829.69	Joback Method
cpg	890.36	J/mol×K	860.52	Joback Method
cpg	904.80	J/mol×K	891.34	Joback Method
cpg	918.34	J/mol×K	922.17	Joback Method
cpg	931.02	J/mol×K	953.00	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U338474&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338474&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.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>

# 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>rinppl:</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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