

# 2,6-Difluoro-3-methylbenzoic acid, 4-tridecyl ester

Inchi:	InChI=1S/C21H32F2O2/c1-4-6-7-8-9-10-11-13-17(12-5-2)25-21(24)19-18(22)15-14-16(3)
InchiKey:	UMICDBBIBQVFEO-UHFFFAOYSA-N
Formula:	C21H32F2O2
SMILES:	CCCCCCCCC(CCC)OC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]:	354.47

## Physical Properties

Property code	Value	Unit	Source
gf	-416.52	kJ/mol	Joback Method
hf	-916.95	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.739		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	2281.00		NIST Webbook
rinpol	2281.00		NIST Webbook
tb	795.89	K	Joback Method
tc	982.92	K	Joback Method
tf	448.75	K	Joback Method
vc	1.157	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.22	J/molxK	795.89	Joback Method
cpg	917.73	J/molxK	827.06	Joback Method
cpg	934.23	J/molxK	858.23	Joback Method
cpg	949.75	J/molxK	889.41	Joback Method
cpg	964.32	J/molxK	920.58	Joback Method
cpg	977.96	J/molxK	951.75	Joback Method
cpg	990.69	J/molxK	982.92	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=U338583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U338583&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>hvap:</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>rinpola:</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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