

# 2,6-Difluorobenzoic acid, hexadecyl ester

**Inchi:** InChI=1S/C23H36F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-27-23(26)22-20(24)17  
**InchiKey:** XZEGTEHJIAIBAM-UHFFFAOYSA-N  
**Formula:** C23H36F2O2  
**SMILES:** CCCCCCCCCCCCCCOC(=O)c1c(F)cccc1F  
**Mol. weight [g/mol]:** 382.53

## Physical Properties

Property code	Value	Unit	Source
gf	-387.61	kJ/mol	Joback Method
hf	-941.48	kJ/mol	Joback Method
hfus	57.54	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.603		Crippen Method
mvol	322.150	ml/mol	McGowan Method
pc	995.76	kPa	Joback Method
rinpol	2457.50		NIST Webbook
rinpol	2457.50		NIST Webbook
tb	837.11	K	Joback Method
tc	1026.91	K	Joback Method
tf	473.77	K	Joback Method
vc	1.276	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.49	J/mol×K	837.11	Joback Method
cpg	1038.69	J/mol×K	868.74	Joback Method
cpg	1055.80	J/mol×K	900.38	Joback Method
cpg	1071.86	J/mol×K	932.01	Joback Method
cpg	1086.90	J/mol×K	963.64	Joback Method
cpg	1100.96	J/mol×K	995.28	Joback Method
cpg	1114.07	J/mol×K	1026.91	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=U292396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292396&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>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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