

# Sarcosine, N-(2,6-difluorobenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C22H33F2NO3/c1-3-4-5-6-7-8-9-10-11-12-16-28-20(26)17-25(2)22(27)21-18(2)
InchiKey:	ZYFRCLRJVJYQWJP-UHFFFAOYSA-N
Formula:	C22H33F2NO3
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	397.50

## Physical Properties

Property code	Value	Unit	Source
gf	-414.17	kJ/mol	Joback Method
hf	-965.89	kJ/mol	Joback Method
hfus	59.57	kJ/mol	Joback Method
hvap	84.48	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.501		Crippen Method
mcvol	319.610	ml/mol	McGowan Method
pc	1102.28	kPa	Joback Method
rinsol	2855.00		NIST Webbook
tb	880.54	K	Joback Method
tc	1079.07	K	Joback Method
tf	544.90	K	Joback Method
vc	1.244	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.19	J/molxK	880.54	Joback Method
cpg	1040.65	J/molxK	913.63	Joback Method
cpg	1055.99	J/molxK	946.72	Joback Method
cpg	1070.24	J/molxK	979.81	Joback Method
cpg	1083.46	J/molxK	1012.89	Joback Method
cpg	1095.69	J/molxK	1045.98	Joback Method
cpg	1106.97	J/molxK	1079.07	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=U321302&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321302&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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