

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

<b>Inchi:</b>	InChI=1S/C26H41F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-32-24(30)21-29(2)2
<b>InchiKey:</b>	IGEJERNJGSPWJH-UHFFFAOYSA-N
<b>Formula:</b>	C26H41F2NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
<b>Mol. weight [g/mol]:</b>	453.61

## Physical Properties

Property code	Value	Unit	Source
gf	-380.49	kJ/mol	Joback Method
hf	-1048.45	kJ/mol	Joback Method
hfus	69.93	kJ/mol	Joback Method
hvap	93.38	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.061		Crippen Method
mcvol	375.970	ml/mol	McGowan Method
pc	867.09	kPa	Joback Method
tb	972.06	K	Joback Method
tc	1193.37	K	Joback Method
tf	589.98	K	Joback Method
vc	1.468	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1270.86	J/molxK	972.06	Joback Method
cpg	1289.08	J/molxK	1008.95	Joback Method
cpg	1305.86	J/molxK	1045.83	Joback Method
cpg	1321.28	J/molxK	1082.72	Joback Method
cpg	1335.40	J/molxK	1119.60	Joback Method
cpg	1348.32	J/molxK	1156.49	Joback Method
cpg	1360.09	J/molxK	1193.37	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=U321305&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321305&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>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>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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