

# D-Alanine, N-(2,6-difluoro-3-methylbenzoyl)-, octadecyl ester

<b>Inchi:</b>	InChI=1S/C29H47F2NO3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-35-29(34)2
<b>InchiKey:</b>	WGOPIBTWJGHGDP-UHFFFAOYSA-N
<b>Formula:</b>	C29H47F2NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1c(F)ccc(C)c1F
<b>Mol. weight [g/mol]:</b>	495.69

## Physical Properties

Property code	Value	Unit	Source
gf	-388.69	kJ/mol	Joback Method
hf	-1141.18	kJ/mol	Joback Method
hfus	75.86	kJ/mol	Joback Method
hvap	104.73	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	8.196		Crippen Method
mcvol	418.240	ml/mol	McGowan Method
pc	740.03	kPa	Joback Method
rinsol	3507.00		NIST Webbook
tb	1082.97	K	Joback Method
tc	1347.91	K	Joback Method
tf	641.50	K	Joback Method
vc	1.647	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1477.16	J/molxK	1082.97	Joback Method
cpg	1495.89	J/molxK	1127.13	Joback Method
cpg	1512.55	J/molxK	1171.28	Joback Method
cpg	1527.25	J/molxK	1215.44	Joback Method
cpg	1540.12	J/molxK	1259.60	Joback Method
cpg	1551.27	J/molxK	1303.75	Joback Method
cpg	1560.83	J/molxK	1347.91	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=U348399&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348399&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mccol:</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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