

# D-Alanine, N-(2,4-difluorobenzoyl)-, eicosyl ester

Inchi:	InChI=1S/C30H49F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-36-30
InchiKey:	FKTOCJQWSMNQOB-UHFFFAOYSA-N
Formula:	C30H49F2NO3
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]:	509.71

## Physical Properties

Property code	Value	Unit	Source
gf	-370.64	kJ/mol	Joback Method
hf	-1150.35	kJ/mol	Joback Method
hfus	78.84	kJ/mol	Joback Method
hvap	106.29	kJ/mol	Joback Method
log10ws	-10.66		Crippen Method
logp	8.668		Crippen Method
mvol	432.330	ml/mol	McGowan Method
pc	708.46	kPa	Joback Method
rinpol	3499.00		NIST Webbook
rinpol	3499.00		NIST Webbook
tb	1100.87	K	Joback Method
tc	1377.70	K	Joback Method
tf	640.25	K	Joback Method
vc	1.702	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1541.79	J/molxK	1100.87	Joback Method
cpg	1561.38	J/molxK	1147.01	Joback Method
cpg	1578.80	J/molxK	1193.15	Joback Method
cpg	1594.19	J/molxK	1239.28	Joback Method
cpg	1607.71	J/molxK	1285.42	Joback Method
cpg	1619.52	J/molxK	1331.56	Joback Method
cpg	1629.79	J/molxK	1377.70	Joback Method

# Sources

<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=U348465&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348465&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>h vap:</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>r in pol:</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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