

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

<b>Inchi:</b>	InChI=1S/C15H19F2NO3/c1-8(2)7-21-15(20)10(4)18-14(19)12-11(16)6-5-9(3)13(12)17/h
<b>InchiKey:</b>	GLJWBLUDHZJNCE-UHFFFAOYSA-N
<b>Formula:</b>	C15H19F2NO3
<b>SMILES:</b>	<chem>Cc1ccc(F)c(C(=O)NC(C)C(=O)OCC(C)C)c1F</chem>
<b>Mol. weight [g/mol]:</b>	299.31

## Physical Properties

Property code	Value	Unit	Source
gf	-509.01	kJ/mol	Joback Method
hf	-857.50	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	73.17	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	2.591		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinsol	2052.00		NIST Webbook
tb	762.21	K	Joback Method
tc	961.93	K	Joback Method
tf	468.72	K	Joback Method
vc	0.857	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	636.07	J/mol×K	762.21	Joback Method
cpg	649.68	J/mol×K	795.50	Joback Method
cpg	662.39	J/mol×K	828.78	Joback Method
cpg	674.23	J/mol×K	862.07	Joback Method
cpg	685.20	J/mol×K	895.36	Joback Method
cpg	695.31	J/mol×K	928.64	Joback Method
cpg	704.59	J/mol×K	961.93	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=U348387&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U348387&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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