

# D-Alanine, N-(2,5-ditrifluoromethylbenzoyl)-, butyl ester

Inchi:	InChI=1S/C16H17F6NO3/c1-3-4-7-26-14(25)9(2)23-13(24)11-8-10(15(17,18)19)5-6-12(1
InchiKey:	OMSCCKDCNAOJGBH-UHFFFAOYSA-N
Formula:	C16H17F6NO3
SMILES:	CCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	385.30

## Physical Properties

Property code	Value	Unit	Source
gf	-1262.08	kJ/mol	Joback Method
hf	-1663.33	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.186		Crippen Method
mcvol	242.150	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	771.17	K	Joback Method
tc	958.69	K	Joback Method
tf	489.67	K	Joback Method
vc	0.969	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.36	J/molxK	771.17	Joback Method
cpg	738.79	J/molxK	802.42	Joback Method
cpg	750.37	J/molxK	833.68	Joback Method
cpg	761.13	J/molxK	864.93	Joback Method
cpg	771.13	J/molxK	896.19	Joback Method
cpg	780.42	J/molxK	927.44	Joback Method
cpg	789.04	J/molxK	958.69	Joback Method

# Sources

<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>
<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=U347799&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U347799&amp;Units=SI</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>rlnpol:</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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