

# D-Alanine, N-(4-ethylbenzoyl)-, hexadecyl ester

<b>Inchi:</b>	InChI=1S/C28H47NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-23-32-28(31)24(3)29-2
<b>InchiKey:</b>	MHTYRACCJITXEY-UHFFFAOYSA-N
<b>Formula:</b>	C28H47NO3
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
<b>Mol. weight [g/mol]:</b>	445.68

## Physical Properties

Property code	Value	Unit	Source
gf	11.77	kJ/mol	Joback Method
hf	-705.38	kJ/mol	Joback Method
hfus	67.89	kJ/mol	Joback Method
hvap	102.81	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	7.392		Crippen Method
mvol	400.610	ml/mol	McGowan Method
pc	835.31	kPa	Joback Method
rinpol	3435.00		NIST Webbook
tb	1051.59	K	Joback Method
tc	1293.59	K	Joback Method
tf	604.01	K	Joback Method
vc	1.554	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.28	J/molxK	1051.59	Joback Method
cpg	1420.56	J/molxK	1091.92	Joback Method
cpg	1437.17	J/molxK	1132.26	Joback Method
cpg	1452.20	J/molxK	1172.59	Joback Method
cpg	1465.75	J/molxK	1212.92	Joback Method
cpg	1477.93	J/molxK	1253.26	Joback Method
cpg	1488.84	J/molxK	1293.59	Joback Method

# Sources

<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=U354097&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U354097&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>

# 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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