

D-Alanine, N-(4-anisoyl)-, butyl ester

Inchi:	InChI=1S/C15H21NO4/c1-4-5-10-20-15(18)11(2)16-14(17)12-6-8-13(19-3)9-7-12/h6-9,1
InchiKey:	AJYRJKIWTNARDY-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	279.33

Physical Properties

Property code	Value	Unit	Source
gf	-202.69	kJ/mol	Joback Method
hf	-569.28	kJ/mol	Joback Method
hfus	35.41	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.157		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinqol	2198.00		NIST Webbook
tb	776.57	K	Joback Method
tc	984.18	K	Joback Method
tf	479.73	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.30	J/molxK	776.57	Joback Method
cpg	663.62	J/molxK	811.17	Joback Method
cpg	676.92	J/molxK	845.77	Joback Method
cpg	689.21	J/molxK	880.38	Joback Method
cpg	700.50	J/molxK	914.98	Joback Method
cpg	710.81	J/molxK	949.58	Joback Method
cpg	720.14	J/molxK	984.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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