

«beta»-Alanine, N-(4-methylbenzoyl)-, butyl ester

Inchi:	InChI=1S/C15H21NO3/c1-3-4-11-19-14(17)9-10-16-15(18)13-7-5-12(2)6-8-13/h5-8H,3-4
InchiKey:	DJALNAQTIZOXKH-UHFFFAOYSA-N
Formula:	C15H21NO3
SMILES:	CCCCOC(=O)CCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	263.33

Physical Properties

Property code	Value	Unit	Source
gf	-95.25	kJ/mol	Joback Method
hf	-431.78	kJ/mol	Joback Method
hfus	37.74	kJ/mol	Joback Method
hvap	74.26	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	2.458		Crippen Method
mcvol	217.440	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2231.00		NIST Webbook
rinpol	2231.00		NIST Webbook
tb	754.59	K	Joback Method
tc	960.29	K	Joback Method
tf	472.50	K	Joback Method
vc	0.833	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.45	J/mol×K	754.59	Joback Method
cpg	635.94	J/mol×K	788.87	Joback Method
cpg	649.47	J/mol×K	823.16	Joback Method
cpg	662.07	J/mol×K	857.44	Joback Method
cpg	673.77	J/mol×K	891.72	Joback Method
cpg	684.59	J/mol×K	926.01	Joback Method
cpg	694.55	J/mol×K	960.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321601&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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