

«beta»-Alanine, N-(4-methoxybenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C23H37NO4/c1-3-4-5-6-7-8-9-10-11-12-19-28-22(25)17-18-24-23(26)20-13-15
InchiKey:	DTLHWNILNUEFOO-UHFFFAOYSA-N
Formula:	C23H37NO4
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	391.54

Physical Properties

Property code	Value	Unit	Source
gf	-132.89	kJ/mol	Joback Method
hf	-729.12	kJ/mol	Joback Method
hfus	59.65	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.279		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
tb	960.05	K	Joback Method
tc	1175.46	K	Joback Method
tf	584.89	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.61	J/molxK	960.05	Joback Method
cpg	1134.57	J/molxK	995.95	Joback Method
cpg	1149.13	J/molxK	1031.85	Joback Method
cpg	1162.33	J/molxK	1067.76	Joback Method
cpg	1174.20	J/molxK	1103.66	Joback Method
cpg	1184.79	J/molxK	1139.56	Joback Method
cpg	1194.13	J/molxK	1175.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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