

«beta»-Alanine, N-(4-butylbenzoyl)-, decyl ester

Inchi:	InChI=1S/C24H39NO3/c1-3-5-7-8-9-10-11-12-20-28-23(26)18-19-25-24(27)22-16-14-21
InchiKey:	ZQXAXGJHMBEQNM-UHFFFAOYSA-N
Formula:	C24H39NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	389.57

Physical Properties

Property code	Value	Unit	Source
gf	-19.47	kJ/mol	Joback Method
hf	-617.54	kJ/mol	Joback Method
hfus	61.05	kJ/mol	Joback Method
hvap	94.29	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.833		Crippen Method
mvol	344.250	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	3373.00		NIST Webbook
rinpol	3373.00		NIST Webbook
tb	960.51	K	Joback Method
tc	1175.99	K	Joback Method
tf	573.93	K	Joback Method
vc	1.337	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.88	J/molxK	960.51	Joback Method
cpg	1167.76	J/molxK	996.42	Joback Method
cpg	1183.34	J/molxK	1032.34	Joback Method
cpg	1197.65	J/molxK	1068.25	Joback Method
cpg	1210.76	J/molxK	1104.16	Joback Method
cpg	1222.74	J/molxK	1140.07	Joback Method
cpg	1233.63	J/molxK	1175.99	Joback Method

Sources

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=U321777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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