

«beta»-Alanine, N-(3-methylbenzoyl)-, undecyl ester

Inchi:	InChI=1S/C22H35NO3/c1-3-4-5-6-7-8-9-10-11-17-26-21(24)15-16-23-22(25)20-14-12-13
InchiKey:	SZYKJFYPIQLDR-UHFFFAOYSA-N
Formula:	C22H35NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(C)c1
Mol. weight [g/mol]:	361.52

Physical Properties

Property code	Value	Unit	Source
gf	-36.31	kJ/mol	Joback Method
hf	-576.26	kJ/mol	Joback Method
hfus	55.87	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.189		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinsol	2990.00		NIST Webbook
tb	914.75	K	Joback Method
tc	1122.55	K	Joback Method
tf	551.39	K	Joback Method
vc	1.224	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.20	J/mol×K	914.75	Joback Method
cpg	1044.50	J/mol×K	949.38	Joback Method
cpg	1059.61	J/mol×K	984.02	Joback Method
cpg	1073.57	J/mol×K	1018.65	Joback Method
cpg	1086.42	J/mol×K	1053.28	Joback Method
cpg	1098.21	J/mol×K	1087.91	Joback Method
cpg	1109.00	J/mol×K	1122.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321634&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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