

«beta»-Alanine, N-(3-methoxybenzoyl)-, decyl ester

Inchi:	InChI=1S/C21H33NO4/c1-3-4-5-6-7-8-9-10-16-26-20(23)14-15-22-21(24)18-12-11-13-19
InchiKey:	VVNBQIGDUHKOFB-UHFFFAOYSA-N
Formula:	C21H33NO4
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	363.49

Physical Properties

Property code	Value	Unit	Source
gf	-149.73	kJ/mol	Joback Method
hf	-687.84	kJ/mol	Joback Method
hfus	54.47	kJ/mol	Joback Method
hvap	90.03	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.499		Crippen Method
mcvol	307.850	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	3039.00		NIST Webbook
tb	914.29	K	Joback Method
tc	1122.24	K	Joback Method
tf	562.35	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.02	J/molxK	914.29	Joback Method
cpg	1012.54	J/molxK	948.95	Joback Method
cpg	1026.79	J/molxK	983.61	Joback Method
cpg	1039.81	J/molxK	1018.27	Joback Method
cpg	1051.64	J/molxK	1052.92	Joback Method
cpg	1062.30	J/molxK	1087.58	Joback Method
cpg	1071.81	J/molxK	1122.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U321713&Units=SI

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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