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

Inchi: InChI=1S/C18H27NO4/c1-3-4-5-6-7-14-23-17(20)12-13-19-18(21)15-8-10-16(22-2)11-9-
InchiKey: OXOLRTPQINANCC-UHFFFAOYSA-N
Formula: C18H27NO4
SMILES: CCCCCCCOC(=O)CCNC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
gf	-174.99	kJ/mol	Joback Method
hf	-625.92	kJ/mol	Joback Method
hfus	46.70	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.329		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	845.65	K	Joback Method
tc	1048.83	K	Joback Method
tf	528.54	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.30	J/mol×K	845.65	Joback Method
cpg	834.18	J/mol×K	879.51	Joback Method
cpg	847.96	J/mol×K	913.38	Joback Method
cpg	860.66	J/mol×K	947.24	Joback Method
cpg	872.29	J/mol×K	981.10	Joback Method
cpg	882.88	J/mol×K	1014.97	Joback Method
cpg	892.45	J/mol×K	1048.83	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=U321825&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume