

«beta»-Alanine, N-(4-methylbenzoyl)-, octyl ester

Inchi:	InChI=1S/C19H29NO3/c1-3-4-5-6-7-8-15-23-18(21)13-14-20-19(22)17-11-9-16(2)10-12-
InchiKey:	KTCFACRDDUARTN-UHFFFAOYSA-N
Formula:	C19H29NO3
SMILES:	CCCCCCCCOC(=O)CCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	319.44

Physical Properties

Property code	Value	Unit	Source
gf	-61.57	kJ/mol	Joback Method
hf	-514.34	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.019		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2646.00		NIST Webbook
tb	846.11	K	Joback Method
tc	1048.85	K	Joback Method
tf	517.58	K	Joback Method
vc	1.056	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.95	J/mol×K	846.11	Joback Method
cpg	864.52	J/mol×K	879.90	Joback Method
cpg	879.02	J/mol×K	913.69	Joback Method
cpg	892.47	J/mol×K	947.48	Joback Method
cpg	904.93	J/mol×K	981.27	Joback Method
cpg	916.42	J/mol×K	1015.06	Joback Method
cpg	926.98	J/mol×K	1048.85	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=U321606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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