

«beta»-Alanine, N-(2-methylbenzoyl)-, hexyl ester

Inchi:	InChI=1S/C17H25NO3/c1-3-4-5-8-13-21-16(19)11-12-18-17(20)15-10-7-6-9-14(15)2/h6-
InchiKey:	JACDKKSFUYFUAI-UHFFFAOYSA-N
Formula:	C17H25NO3
SMILES:	CCCCCOC(=O)CCNC(=O)c1ccccc1C
Mol. weight [g/mol]:	291.39

Physical Properties

Property code	Value	Unit	Source
gf	-78.41	kJ/mol	Joback Method
hf	-473.06	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	78.71	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.238		Crippen Method
mcvol	245.620	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2354.00		NIST Webbook
tb	800.35	K	Joback Method
tc	1003.35	K	Joback Method
tf	495.04	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.33	J/molxK	800.35	Joback Method
cpg	748.41	J/molxK	834.18	Joback Method
cpg	762.47	J/molxK	868.02	Joback Method
cpg	775.56	J/molxK	901.85	Joback Method
cpg	787.69	J/molxK	935.68	Joback Method
cpg	798.90	J/molxK	969.52	Joback Method
cpg	809.22	J/molxK	1003.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321617&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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