D-Alanine, N-(4-butylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H31NO3/c1-4-6-8-9-15-24-20(23)16(3)21-19(22)18-13-11-17(12-14-18)10-
InchiKey: FNTCXASHEVHNLQ-UHFFFAOYSA-N
Formula: C20H31NO3
SMILES: CCCCCCOC(=O)C(C)NC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 333.46

Physical Properties

Property code	Value	Unit	Source
gf	-55.59	kJ/mol	Joback Method
hf	-540.26	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	85.00	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.271		Crippen Method
mcvol	287.890	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2623.00		NIST Webbook
tb	868.55	K	Joback Method
tc	1073.74	K	Joback Method
tf	513.85	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.49	J/mol×K	868.55	Joback Method
cpg	924.40	J/mol×K	902.75	Joback Method
cpg	939.17	J/mol×K	936.95	Joback Method
cpg	952.84	J/mol×K	971.14	Joback Method
cpg	965.45	J/mol×K	1005.34	Joback Method
cpg	977.04	J/mol×K	1039.54	Joback Method
cpg	987.66	J/mol×K	1073.74	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=U354101&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