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

Inchi: InChI=1S/C29H49NO3/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-24-33-29(32)25(3)30-28(

InchiKey: PTPLVYOEOJGLJE-UHFFFAOYSA-N

Formula: C29H49NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CCCC)cc1

Mol. weight [g/mol]: 459.70

Physical Properties

Property code	Value	Unit	Source
gf	20.19	kJ/mol	Joback Method
hf	-726.02	kJ/mol	Joback Method
hfus	70.48	kJ/mol	Joback Method
hvap	105.04	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	7.782		Crippen Method
mcvol	414.700	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	3543.00		NIST Webbook
tb	1074.47	K	Joback Method
tc	1326.16	K	Joback Method
tf	615.28	K	Joback Method
vc	1.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.98	J/mol×K	1074.47	Joback Method
cpg	1484.75	J/mol×K	1116.42	Joback Method
cpg	1501.71	J/mol×K	1158.37	Joback Method
cpg	1516.99	J/mol×K	1200.31	Joback Method
cpg	1530.71	J/mol×K	1242.26	Joback Method
cpg	1542.99	J/mol×K	1284.21	Joback Method
cpg	1553.95	J/mol×K	1326.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354105&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume