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

Inchi: InChI=1S/C27H45NO3/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-22-31-27(30)23(3)28-26(2

InchiKey: ZZGOZBLQSXFELC-UHFFFAOYSA-N

Formula: C27H45NO3

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

Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	3.35	kJ/mol	Joback Method
hf	-684.74	kJ/mol	Joback Method
hfus	65.30	kJ/mol	Joback Method
hvap	100.58	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	7.002		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	883.67	kPa	Joback Method
rinpol	3336.00		NIST Webbook
tb	1028.71	K	Joback Method
tc	1262.34	K	Joback Method
tf	592.74	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.91	J/mol×K	1028.71	Joback Method
cpg	1356.77	J/mol×K	1067.65	Joback Method
cpg	1373.06	J/mol×K	1106.59	Joback Method
cpg	1387.86	J/mol×K	1145.53	Joback Method
cpg	1401.27	J/mol×K	1184.46	Joback Method
cpg	1413.36	J/mol×K	1223.40	Joback Method
cpg	1424.23	J/mol×K	1262.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354096&Units=SI
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

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