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

Inchi: InChI=1S/C23H37NO3/c1-4-6-7-8-9-10-11-12-13-18-27-23(26)19(3)24-22(25)21-16-14-2
InchiKey: GCJQCZNTJKTDHF-UHFFFAOYSA-N
Formula: C23H37NO3
SMILES: CCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
gf	-30.33	kJ/mol	Joback Method
hf	-602.18	kJ/mol	Joback Method
hfus	54.94	kJ/mol	Joback Method
hvap	91.68	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.441		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	937.19	K	Joback Method
tc	1148.84	K	Joback Method
tf	547.66	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.68	J/mol×K	937.19	Joback Method
cpg	1106.26	J/mol×K	972.47	Joback Method
cpg	1121.57	J/mol×K	1007.74	Joback Method
cpg	1135.67	J/mol×K	1043.02	Joback Method
cpg	1148.59	J/mol×K	1078.29	Joback Method
cpg	1160.40	J/mol×K	1113.57	Joback Method
cpg	1171.15	J/mol×K	1148.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354092&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
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
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