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

Inchi: InChI=1S/C25H41NO3/c1-4-6-7-8-9-10-11-12-13-14-15-20-29-25(28)21(3)26-24(27)23-1
InchiKey: RFOAMGMVCXIRJL-UHFFFAOYSA-N
Formula: C25H41NO3
SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	-13.49	kJ/mol	Joback Method
hf	-643.46	kJ/mol	Joback Method
hfus	60.12	kJ/mol	Joback Method
hvap	96.13	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.222		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	993.88	kPa	Joback Method
rinpol	3130.00		NIST Webbook
tb	982.95	K	Joback Method
tc	1203.45	K	Joback Method
tf	570.20	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.37	J/mol×K	982.95	Joback Method
cpg	1230.52	J/mol×K	1019.70	Joback Method
cpg	1246.26	J/mol×K	1056.45	Joback Method
cpg	1260.67	J/mol×K	1093.20	Joback Method
cpg	1273.82	J/mol×K	1129.95	Joback Method
cpg	1285.77	J/mol×K	1166.70	Joback Method
cpg	1296.58	J/mol×K	1203.45	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=U354094&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