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

Inchi: InChI=1S/C22H35NO3/c1-4-6-7-8-9-10-11-12-17-26-22(25)18(3)23-21(24)20-15-13-19(5
InchiKey: CGYHOQUMOMWVQF-UHFFFAOYSA-N
Formula: C22H35NO3
SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 361.52

Physical Properties

Property code	Value	Unit	Source
gf	-38.75	kJ/mol	Joback Method
hf	-581.54	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	89.45	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.051		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2827.00		NIST Webbook
tb	914.31	K	Joback Method
tc	1122.96	K	Joback Method
tf	536.39	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.65	J/mol×K	914.31	Joback Method
cpg	1044.99	J/mol×K	949.09	Joback Method
cpg	1060.11	J/mol×K	983.86	Joback Method
cpg	1074.06	J/mol×K	1018.64	Joback Method
cpg	1086.88	J/mol×K	1053.41	Joback Method
cpg	1098.63	J/mol×K	1088.19	Joback Method
cpg	1109.34	J/mol×K	1122.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354091&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