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

Inchi: InChI=1S/C21H33NO3/c1-4-6-7-8-9-10-11-16-25-21(24)17(3)22-20(23)19-14-12-18(5-2)
InchiKey: XNRVZSHIVHWFHC-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-47.17	kJ/mol	Joback Method
hf	-560.90	kJ/mol	Joback Method
hfus	49.76	kJ/mol	Joback Method
hvap	87.23	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	4.661		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2725.00		NIST Webbook
tb	891.43	K	Joback Method
tc	1097.95	K	Joback Method
tf	525.12	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.24	J/mol×K	891.43	Joback Method
cpg	984.36	J/mol×K	925.85	Joback Method
cpg	999.30	J/mol×K	960.27	Joback Method
cpg	1013.11	J/mol×K	994.69	Joback Method
cpg	1025.83	J/mol×K	1029.11	Joback Method
cpg	1037.50	J/mol×K	1063.53	Joback Method
cpg	1048.17	J/mol×K	1097.95	Joback Method

Sources

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=U354090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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