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

Inchi: InChI=1S/C19H29NO3/c1-4-6-7-8-9-14-23-19(22)15(3)20-18(21)17-12-10-16(5-2)11-13-
InchiKey: FICDLRMHBLQLBR-UHFFFAOYSA-N
Formula: C19H29NO3
SMILES: CCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 319.44

Physical Properties

Property code	Value	Unit	Source
gf	-64.01	kJ/mol	Joback Method
hf	-519.62	kJ/mol	Joback Method
hfus	44.58	kJ/mol	Joback Method
hvap	82.78	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	3.881		Crippen Method
mcvol	273.800	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2527.00		NIST Webbook
tb	845.67	K	Joback Method
tc	1050.28	K	Joback Method
tf	502.58	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.47	J/mol×K	845.67	Joback Method
cpg	865.17	J/mol×K	879.77	Joback Method
cpg	879.77	J/mol×K	913.87	Joback Method
cpg	893.29	J/mol×K	947.97	Joback Method
cpg	905.79	J/mol×K	982.08	Joback Method
cpg	917.29	J/mol×K	1016.18	Joback Method
cpg	927.84	J/mol×K	1050.28	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=U354089&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

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