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

Inchi: InChI=1S/C18H27NO3/c1-5-15-8-10-16(11-9-15)17(20)19-14(4)18(21)22-12-6-7-13(2)3/l
InchiKey: UFTBUEAUQACHEZ-UHFFFAOYSA-N
Formula: C18H27NO3
SMILES: CCc1ccc(C(=O)NC(C)C(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]: 305.41

Physical Properties

Property code	Value	Unit	Source
gf	-74.87	kJ/mol	Joback Method
hf	-504.26	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.347		Crippen Method
mcvol	259.710	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	2375.00		NIST Webbook
tb	822.35	K	Joback Method
tc	1029.42	K	Joback Method
tf	476.31	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	791.78	J/mol×K	822.35	Joback Method
cpg	807.44	J/mol×K	856.86	Joback Method
cpg	821.98	J/mol×K	891.37	Joback Method
cpg	835.45	J/mol×K	925.88	Joback Method
cpg	847.88	J/mol×K	960.39	Joback Method
cpg	859.30	J/mol×K	994.91	Joback Method
cpg	869.75	J/mol×K	1029.42	Joback Method

Sources

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=U354087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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