D-Alanine, N-(3-anisoyl)-, isohexyl ester

Inchi: InChI=1S/C17H25NO4/c1-12(2)7-6-10-22-17(20)13(3)18-16(19)14-8-5-9-15(11-14)21-4/h
InchiKey: KFDHKVWDDUDRNC-UHFFFAOYSA-N
Formula: C17H25NO4
SMILES: COc1cccc(C(=O)NC(C)C(=O)OCCCC(C)C)c1
Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-188.29	kJ/mol	Joback Method
hf	-615.84	kJ/mol	Joback Method
hfus	37.06	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	2.793		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	2390.00		NIST Webbook
tb	821.89	K	Joback Method
tc	1029.57	K	Joback Method
tf	487.27	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.65	J/mol×K	821.89	Joback Method
cpg	777.62	J/mol×K	856.50	Joback Method
cpg	791.45	J/mol×K	891.12	Joback Method
cpg	804.18	J/mol×K	925.73	Joback Method
cpg	815.81	J/mol×K	960.34	Joback Method
cpg	826.36	J/mol×K	994.96	Joback Method
cpg	835.86	J/mol×K	1029.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354045&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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