D-Alanine, N-(4-anisoyl)-, isobutyl ester

Inchi: InChI=1S/C15H21NO4/c1-10(2)9-20-15(18)11(3)16-14(17)12-5-7-13(19-4)8-6-12/h5-8,10
InchiKey: XYZZSWJUIGNJEC-UHFFFAOYSA-N
Formula: C15H21NO4
SMILES: COc1ccc(C(=O)NC(C)C(=O)OCC(C)C)cc1
Mol. weight [g/mol]: 279.33

Physical Properties

Property code	Value	Unit	Source
gf	-205.13	kJ/mol	Joback Method
hf	-574.56	kJ/mol	Joback Method
hfus	31.89	kJ/mol	Joback Method
hvap	75.89	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.013		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	776.13	K	Joback Method
tc	986.73	K	Joback Method
tf	464.73	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.86	J/mol×K	776.13	Joback Method
cpg	664.39	J/mol×K	811.23	Joback Method
cpg	677.86	J/mol×K	846.33	Joback Method
cpg	690.27	J/mol×K	881.43	Joback Method
cpg	701.65	J/mol×K	916.53	Joback Method
cpg	712.01	J/mol×K	951.63	Joback Method
cpg	721.36	J/mol×K	986.73	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=U348487&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