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

Inchi: InChI=1S/C19H29NO4/c1-4-5-6-7-8-9-13-24-19(22)15(2)20-18(21)16-11-10-12-17(14-16
InchiKey: FCKLLKQLHULSHW-UHFFFAOYSA-N
Formula: C19H29NO4
SMILES: CCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 335.44

Physical Properties

Property code	Value	Unit	Source
gf	-169.01	kJ/mol	Joback Method
hf	-651.84	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	85.19	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.717		Crippen Method
mcvol	279.670	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2642.00		NIST Webbook
tb	868.09	K	Joback Method
tc	1073.67	K	Joback Method
tf	524.81	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.35	J/mol×K	868.09	Joback Method
cpg	893.55	J/mol×K	902.35	Joback Method
cpg	907.56	J/mol×K	936.62	Joback Method
cpg	920.42	J/mol×K	970.88	Joback Method
cpg	932.15	J/mol×K	1005.14	Joback Method
cpg	942.77	J/mol×K	1039.41	Joback Method
cpg	952.31	J/mol×K	1073.67	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=U354047&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