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

Inchi: InChI=1S/C26H43NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-20-31-26(29)22(2)27-25(28
InchiKey: CWKOORSTSZMDQA-UHFFFAOYSA-N
Formula: C26H43NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 433.62

Physical Properties

Property code	Value	Unit	Source
gf	-110.07	kJ/mol	Joback Method
hf	-796.32	kJ/mol	Joback Method
hfus	63.90	kJ/mol	Joback Method
hvap	100.77	kJ/mol	Joback Method
log10ws	-8.03		Crippen Method
logp	6.448		Crippen Method
mcvol	378.300	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	1028.25	K	Joback Method
tc	1261.50	K	Joback Method
tf	603.70	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1304.79	J/mol×K	1028.25	Joback Method
cpg	1321.43	J/mol×K	1067.13	Joback Method
cpg	1336.35	J/mol×K	1106.00	Joback Method
cpg	1349.62	J/mol×K	1144.88	Joback Method
cpg	1361.30	J/mol×K	1183.75	Joback Method
cpg	1371.46	J/mol×K	1222.63	Joback Method
cpg	1380.16	J/mol×K	1261.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354053&Units=SI

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