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

Inchi: InChI=1S/C28H47NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-33-28(31)24(2)29
InchiKey: LPPHJEXVRAJZKH-UHFFFAOYSA-N
Formula: C28H47NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]: 461.68

Physical Properties

Property code	Value	Unit	Source
gf	-93.23	kJ/mol	Joback Method
hf	-837.60	kJ/mol	Joback Method
hfus	69.08	kJ/mol	Joback Method
hvap	105.22	kJ/mol	Joback Method
log10ws	-8.86		Crippen Method
logp	7.228		Crippen Method
mcvol	406.480	ml/mol	McGowan Method
pc	827.16	kPa	Joback Method
rinpol	3526.00		NIST Webbook
tb	1074.01	K	Joback Method
tc	1325.04	K	Joback Method
tf	626.24	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1430.42	J/mol×K	1074.01	Joback Method
cpg	1447.66	J/mol×K	1115.85	Joback Method
cpg	1462.89	J/mol×K	1157.69	Joback Method
cpg	1476.23	J/mol×K	1199.52	Joback Method
cpg	1487.74	J/mol×K	1241.36	Joback Method
cpg	1497.53	J/mol×K	1283.20	Joback Method
cpg	1505.69	J/mol×K	1325.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348500&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

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