

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

Inchi: InChI=1S/C25H41NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-30-25(28)21(2)26-24(27)22
InchiKey: FVNQLLQISSSIFV-UHFFFAOYSA-N
Formula: C25H41NO4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 419.60

Physical Properties

Property code	Value	Unit	Source
gf	-118.49	kJ/mol	Joback Method
hf	-775.68	kJ/mol	Joback Method
hfus	61.31	kJ/mol	Joback Method
hvap	98.54	kJ/mol	Joback Method
log10ws	-7.61		Crippen Method
logp	6.058		Crippen Method
mcvol	364.210	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	1005.37	K	Joback Method
tc	1231.61	K	Joback Method
tf	592.43	K	Joback Method
vc	1.405	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1242.47	J/mol×K	1005.37	Joback Method
cpg	1258.85	J/mol×K	1043.08	Joback Method
cpg	1273.62	J/mol×K	1080.78	Joback Method
cpg	1286.85	J/mol×K	1118.49	Joback Method
cpg	1298.58	J/mol×K	1156.20	Joback Method
cpg	1308.88	J/mol×K	1193.90	Joback Method
cpg	1317.79	J/mol×K	1231.61	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=U354052&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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