D-Alanine, N-ethoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C22H43NO4/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-27-21(24)20(3)23-2
InchiKey: MUGABKIZWOIKQE-UHFFFAOYSA-N
Formula: C22H43NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)N=C(O)OCC
Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
hf	-959.51	kJ/mol	Joback Method
hvap	95.82	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	6.350		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	917.72	kPa	Joback Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		NIST Webbook
tb	969.77	K	Joback Method
tc	1192.79	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U347759&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

hf: Enthalpy of formation 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