D-Alanine, N-butoxycarbonyl-, decyl ester

Inchi: InChI=1S/C18H35NO4/c1-4-6-8-9-10-11-12-13-15-22-17(20)16(3)19-18(21)23-14-7-5-2/h
InchiKey: ASRYTBCXTNSWSI-UHFFFAOYSA-N
Formula: C18H35NO4
SMILES: CCCCCCCCCCOC(=O)C(C)N=C(O)OCCCC
Mol. weight [g/mol]: 329.47

Physical Properties

Property code	Value	Unit	Source
hf	-876.95	kJ/mol	Joback Method
hvap	86.91	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.790		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1175.24	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	878.25	K	Joback Method
tc	1075.49	K	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=U347724&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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