D-Homophenylalanine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C18H27NO4/c1-5-22-18(21)19-16(17(20)23-14(4)13(2)3)12-11-15-9-7-6-8-10-
InchiKey: CLNFJLQNJRIWKG-IURRXHLWSA-N
Formula: C18H27NO4
SMILES: CCOC(O)=NC(CCc1ccccc1)C(=O)OC(C)C(C)C
Mol. weight [g/mol]: 321.41

Physical Properties

Property code	Value	Unit	Source
hf	-650.98	kJ/mol	Joback Method
hvap	88.41	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.526		Crippen Method
mcvol	265.580	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2160.90		NIST Webbook
rinpol	2160.90		NIST Webbook
tb	904.05	K	Joback Method
tc	1116.00	K	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=R501841&Units=SI

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