D-«alpha»-Aminoadipic acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C19H35NO6/c1-8-24-19(23)20-16(18(22)26-15(7)13(4)5)10-9-11-17(21)25-14(

InchiKey: UAFHTPVFKRVEM-YOFGXBMJSA-N

Formula: C19H35NO6

SMILES: CCOC(=O)NC(CCCC(=O)OC(C)C(C)C)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 373.48

Physical Properties

Property code	Value	Unit	Source
hfus	40.81	kJ/mol	Joback Method
logp	3.447		Crippen Method
mcvol	310.870	ml/mol	McGowan Method
rinpol	2250.70		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.52	J/mol×K	910.96	Joback Method
cpg	1039.96	J/mol×K	945.25	Joback Method
cpg	1053.99	J/mol×K	979.54	Joback Method
cpg	1066.62	J/mol×K	1013.83	Joback Method
cpg	1077.87	J/mol×K	1048.12	Joback Method
cpg	1087.74	J/mol×K	1082.41	Joback Method
cpg	1096.24	J/mol×K	1116.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R501747&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices