L-Alanine, N-(3-cyclopentylpropionyl)-, methyl ester

Inchi: InChI=1S/C12H21NO3/c1-9(12(15)16-2)13-11(14)8-7-10-5-3-4-6-10/h9-10H,3-8H2,1-2H

InchiKey: ZUFRPVZUKJBNJQ-UHFFFAOYSA-N

Formula: C12H21NO3

SMILES: COC(=O)C(C)NC(=O)CCC1CCCC1

Mol. weight [g/mol]: 227.30

Physical Properties

Property code	Value	Unit	Source
hfus	26.73	kJ/mol	Joback Method
logp	1.635		Crippen Method
mcvol	188.070	ml/mol	McGowan Method
rinpol	1712.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	558.82	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.51	J/mol×K	669.13	Joback Method
cpg	551.07	J/mol×K	703.21	Joback Method
cpg	566.62	J/mol×K	737.30	Joback Method
cpg	581.21	J/mol×K	771.38	Joback Method
cpg	594.83	J/mol×K	805.47	Joback Method
cpg	607.54	J/mol×K	839.55	Joback Method
cpg	619.34	J/mol×K	873.64	Joback Method

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299651&Units=SI

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

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

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
tb:	Normal Boiling Point Temperature