3-cyclopentylpropionic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H28O2/c1-4-5-10-16(13-14(2)3)19-17(18)12-11-15-8-6-7-9-15/h14-16H,4,6

InchiKey: AJIYNFIZBQJLGY-UHFFFAOYSA-N

Formula: C17H28O2

SMILES: CCC#CC(CC(C)C)OC(=O)CCC1CCCC1

Mol. weight [g/mol]: 264.41

Physical Properties

Property code	Value	Unit	Source
hfus	32.58	kJ/mol	Joback Method
logp	4.328		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
rinpol	1787.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.06	J/mol×K	688.05	Joback Method
cpg	703.51	J/mol×K	722.68	Joback Method
cpg	722.76	J/mol×K	757.31	Joback Method
cpg	740.86	J/mol×K	791.94	Joback Method
cpg	757.83	J/mol×K	826.57	Joback Method
cpg	773.71	J/mol×K	861.20	Joback Method
cpg	788.53	J/mol×K	895.84	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=U292469&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