3-cyclopentylpropionic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C13H22O2/c1-11(2)9-10-15-13(14)8-7-12-5-3-4-6-12/h9,12H,3-8,10H2,1-2H3

InchiKey: YSICNKUSJOTUON-UHFFFAOYSA-N

Formula: C13H22O2

SMILES: CC(C)=CCOC(=O)CCC1CCCC1

Mol. weight [g/mol]: 210.32

Physical Properties

Property code	Value	Unit	Source
hfus	25.04	kJ/mol	Joback Method
logp	3.466		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	542.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.03	J/mol×K	592.45	Joback Method
cpg	503.58	J/mol×K	626.06	Joback Method
cpg	521.12	J/mol×K	659.67	Joback Method
cpg	537.67	J/mol×K	693.28	Joback Method
cpg	553.28	J/mol×K	726.89	Joback Method
cpg	567.98	J/mol×K	760.50	Joback Method
cpg	581.82	J/mol×K	794.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292465&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
tb:	Normal Boiling Point Temperature