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]: 210.31

Physical Properties

Property code	Value	Unit	Source
gf	-67.12	kJ/mol	Joback Method
hf	-388.54	kJ/mol	Joback Method
hfus	25.04	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	3.466		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	1549.00		NIST Webbook
rinpol	1549.00		NIST Webbook
tb	592.45	K	Joback Method
tc	794.12	K	Joback Method
tf	300.29	K	Joback Method
vc	0.710	m3/kmol	Joback Method

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

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=U292465&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume