3-Cyclopentylpropionic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H18O2/c1-2-3-6-11-15-13(14)10-9-12-7-4-5-8-12/h1,3,6,12H,4-5,7-11H2/b

InchiKey: PVKOVMPZAUYZTO-ZZXKWVIFSA-N

Formula: C13H18O2

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

Mol. weight [g/mol]: 206.28

Physical Properties

Property code	Value	Unit	Source
gf	164.50	kJ/mol	Joback Method
hf	-86.85	kJ/mol	Joback Method
hfus	29.32	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.689		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1578.60		NIST Webbook
rinpol	1578.60		NIST Webbook
tb	582.69	K	Joback Method
tc	794.19	K	Joback Method
tf	361.22	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.69	J/mol×K	582.69	Joback Method
cpg	461.03	J/mol×K	617.94	Joback Method
cpg	477.33	J/mol×K	653.19	Joback Method
cpg	492.64	J/mol×K	688.44	Joback Method
cpg	507.01	J/mol×K	723.69	Joback Method
cpg	520.49	J/mol×K	758.94	Joback Method
cpg	533.12	J/mol×K	794.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292466&Units=SI
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

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