3-Cyclopentylpropionic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H22O2/c1-3-7-13(4-2)16-14(15)11-10-12-8-5-6-9-12/h12-13H,4-6,8-11H2,1

InchiKey: BDPKCKWTSQVSMQ-UHFFFAOYSA-N

Formula: C14H22O2

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

Mol. weight [g/mol]: 222.32

Physical Properties

Property code	Value	Unit	Source
gf	69.99	kJ/mol	Joback Method
hf	-249.59	kJ/mol	Joback Method
hfus	28.34	kJ/mol	Joback Method
hvap	57.94	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.302		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1605.00		NIST Webbook
tb	619.85	K	Joback Method
tc	833.36	K	Joback Method
tf	421.70	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.77	J/mol×K	619.85	Joback Method
cpg	537.97	J/mol×K	655.43	Joback Method
cpg	556.08	J/mol×K	691.02	Joback Method
cpg	573.12	J/mol×K	726.60	Joback Method
cpg	589.14	J/mol×K	762.19	Joback Method
cpg	604.14	J/mol×K	797.77	Joback Method
cpg	618.18	J/mol×K	833.36	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=U292467&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