3-Cyclopentylpropionic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C12H18O2/c1-3-10(2)14-12(13)9-8-11-6-4-5-7-11/h1,10-11H,4-9H2,2H3
InchiKey: WEHCCFDMIBZMBC-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: C#CC(C)OC(=O)CCC1CCCC1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	73.42	kJ/mol	Joback Method
hf	-188.71	kJ/mol	Joback Method
hfus	23.01	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.522		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1367.10		NIST Webbook
rinpol	1367.10		NIST Webbook
tb	555.21	K	Joback Method
tc	765.49	K	Joback Method
tf	340.03	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.64	J/mol×K	555.21	Joback Method
cpg	431.26	J/mol×K	590.26	Joback Method
cpg	447.88	J/mol×K	625.30	Joback Method
cpg	463.54	J/mol×K	660.35	Joback Method
cpg	478.28	J/mol×K	695.40	Joback Method
cpg	492.12	J/mol×K	730.44	Joback Method
cpg	505.09	J/mol×K	765.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292464&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

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