4-Oxo-4-phenylbutyric acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C14H14O3/c1-3-11(2)17-14(16)10-9-13(15)12-7-5-4-6-8-12/h1,4-8,11H,9-10H2

InchiKey: LPQSZKLNDUYKJD-UHFFFAOYSA-N

Formula: C14H14O3

SMILES: C#CC(C)OC(=O)CCC(=O)c1ccccc1

Mol. weight [g/mol]: 230.26

Physical Properties

Property code	Value	Unit	Source
gf	37.20	kJ/mol	Joback Method
hf	-166.52	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.214		Crippen Method
mcvol	184.770	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	666.24	K	Joback Method
tc	890.13	K	Joback Method
tf	428.02	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.76	J/mol×K	666.24	Joback Method
cpg	482.79	J/mol×K	703.55	Joback Method
cpg	495.84	J/mol×K	740.87	Joback Method
cpg	507.94	J/mol×K	778.18	Joback Method
cpg	519.13	J/mol×K	815.50	Joback Method
cpg	529.45	J/mol×K	852.81	Joback Method
cpg	538.95	J/mol×K	890.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406982&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