Butyric acid, 2-phenyl-, but-3-yn-2-yl ester

Inchi: InChI=1S/C14H16O2/c1-4-11(3)16-14(15)13(5-2)12-9-7-6-8-10-12/h1,6-11,13H,5H2,2-3H

InchiKey: DXKZGGUUTWOREF-UHFFFAOYSA-N

Formula: C14H16O2

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

Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	163.68	kJ/mol	Joback Method
hf	-59.22	kJ/mol	Joback Method
hfus	24.77	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.745		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1460.00		NIST Webbook
rinpol	1460.00		NIST Webbook
tb	611.93	K	Joback Method
tc	833.72	K	Joback Method
tf	363.09	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.96	J/mol×K	611.93	Joback Method
cpg	467.97	J/mol×K	648.89	Joback Method
cpg	482.94	J/mol×K	685.86	Joback Method
cpg	496.91	J/mol×K	722.82	Joback Method
cpg	509.92	J/mol×K	759.79	Joback Method
cpg	522.02	J/mol×K	796.75	Joback Method
cpg	533.24	J/mol×K	833.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406914&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