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

Inchi: InChI=1S/C13H14O2/c1-3-11(2)15-13(14)10-9-12-7-5-4-6-8-12/h1,4-8,11H,9-10H2,2H3
InchiKey: APZMFOKMZRKWPN-UHFFFAOYSA-N
Formula: C13H14O2
SMILES: C#CC(C)OC(=O)CCc1ccccc1
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	157.70	kJ/mol	Joback Method
hf	-33.30	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.184		Crippen Method
mcvol	169.110	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1440.00		NIST Webbook
tb	589.49	K	Joback Method
tc	810.67	K	Joback Method
tf	366.82	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.50	J/mol×K	589.49	Joback Method
cpg	417.51	J/mol×K	626.35	Joback Method
cpg	431.56	J/mol×K	663.22	Joback Method
cpg	444.68	J/mol×K	700.08	Joback Method
cpg	456.93	J/mol×K	736.94	Joback Method
cpg	468.32	J/mol×K	773.80	Joback Method
cpg	478.90	J/mol×K	810.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299172&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