3-Phenylpropionic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C14H14O2/c1-2-3-7-12-16-14(15)11-10-13-8-5-4-6-9-13/h1,3-9H,10-12H2
InchiKey: YFHXFLJONGJWOS-UHFFFAOYSA-N
Formula: C14H14O2
SMILES: C#CC=CCOC(=O)CCc1ccccc1
Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	248.78	kJ/mol	Joback Method
hf	68.56	kJ/mol	Joback Method
hfus	32.02	kJ/mol	Joback Method
hvap	58.01	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.352		Crippen Method
mcvol	178.900	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	616.97	K	Joback Method
tc	838.88	K	Joback Method
tf	388.01	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.33	J/mol×K	616.97	Joback Method
cpg	445.03	J/mol×K	653.96	Joback Method
cpg	458.75	J/mol×K	690.94	Joback Method
cpg	471.54	J/mol×K	727.93	Joback Method
cpg	483.45	J/mol×K	764.91	Joback Method
cpg	494.54	J/mol×K	801.90	Joback Method
cpg	504.87	J/mol×K	838.88	Joback Method

Sources

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=U299173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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