Phenylacetic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H12O2/c1-2-3-7-10-15-13(14)11-12-8-5-4-6-9-12/h1,3-9H,10-11H2/b7-3+
InchiKey: GHMVFRGXYGUKSY-XVNBXDOJSA-N
Formula: C13H12O2
SMILES: C#CC=CCOC(=O)Cc1ccccc1
Mol. weight [g/mol]: 200.23

Physical Properties

Property code	Value	Unit	Source
gf	240.36	kJ/mol	Joback Method
hf	89.20	kJ/mol	Joback Method
hfus	29.43	kJ/mol	Joback Method
hvap	55.78	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	1.962		Crippen Method
mcvol	164.810	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1586.40		NIST Webbook
rinpol	1586.40		NIST Webbook
tb	594.09	K	Joback Method
tc	820.19	K	Joback Method
tf	376.74	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.89	J/mol×K	594.09	Joback Method
cpg	395.94	J/mol×K	631.77	Joback Method
cpg	409.02	J/mol×K	669.46	Joback Method
cpg	421.19	J/mol×K	707.14	Joback Method
cpg	432.50	J/mol×K	744.83	Joback Method
cpg	443.01	J/mol×K	782.51	Joback Method
cpg	452.77	J/mol×K	820.19	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=U292611&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