Phenylacetic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H16O2/c1-3-8-13(4-2)16-14(15)11-12-9-6-5-7-10-12/h5-7,9-10,13H,4,11H2
InchiKey: MTKBAYZOWSPANS-UHFFFAOYSA-N
Formula: C14H16O2
SMILES: CC#CC(CC)OC(=O)Cc1ccccc1
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	145.85	kJ/mol	Joback Method
hf	-73.54	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.574		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1602.80		NIST Webbook
tb	631.25	K	Joback Method
tc	858.83	K	Joback Method
tf	437.22	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.49	J/mol×K	631.25	Joback Method
cpg	469.63	J/mol×K	669.18	Joback Method
cpg	484.73	J/mol×K	707.11	Joback Method
cpg	498.83	J/mol×K	745.04	Joback Method
cpg	511.96	J/mol×K	782.97	Joback Method
cpg	524.16	J/mol×K	820.90	Joback Method
cpg	535.44	J/mol×K	858.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292532&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