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

Inchi: InChI=1S/C15H18O2/c1-3-8-14(4-2)17-15(16)12-11-13-9-6-5-7-10-13/h5-7,9-10,14H,4,1
InchiKey: RLHCYVPRHPXILZ-UHFFFAOYSA-N
Formula: C15H18O2
SMILES: CC#CC(CC)OC(=O)CCc1ccccc1
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	154.27	kJ/mol	Joback Method
hf	-94.18	kJ/mol	Joback Method
hfus	31.03	kJ/mol	Joback Method
hvap	62.18	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.964		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	654.13	K	Joback Method
tc	877.48	K	Joback Method
tf	448.49	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.64	J/mol×K	654.13	Joback Method
cpg	521.28	J/mol×K	691.36	Joback Method
cpg	536.86	J/mol×K	728.58	Joback Method
cpg	551.42	J/mol×K	765.81	Joback Method
cpg	564.99	J/mol×K	803.03	Joback Method
cpg	577.59	J/mol×K	840.26	Joback Method
cpg	589.28	J/mol×K	877.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299174&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