1-Phenyl-3-ethyl-4-hexen-1-yn-3-ol

Inchi: InChI=1S/C14H16O/c1-3-11-14(15,4-2)12-10-13-8-6-5-7-9-13/h3,5-9,11,15H,4H2,1-2H3/
InchiKey: LUVLOEMXAFKSFO-QDEBKDIKSA-N
Formula: C14H16O
SMILES: CC=CC(O)(C#Cc1ccccc1)CC
Mol. weight [g/mol]: 200.28

Physical Properties

Property code	Value	Unit	Source
gf	328.45	kJ/mol	Joback Method
hf	132.78	kJ/mol	Joback Method
hfus	26.06	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.755		Crippen Method
mcvol	177.330	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook
tb	648.51	K	Joback Method
tc	871.45	K	Joback Method
tf	438.22	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.62	J/mol×K	648.51	Joback Method
cpg	461.97	J/mol×K	685.67	Joback Method
cpg	475.30	J/mol×K	722.82	Joback Method
cpg	487.71	J/mol×K	759.98	Joback Method
cpg	499.27	J/mol×K	797.13	Joback Method
cpg	510.09	J/mol×K	834.29	Joback Method
cpg	520.24	J/mol×K	871.45	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=R419133&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