1-(Phenylethynyl)-1-cyclopentanol

Inchi: InChI=1S/C13H14O/c14-13(9-4-5-10-13)11-8-12-6-2-1-3-7-12/h1-3,6-7,14H,4-5,9-10H2
InchiKey: ZDUXLFHBOAAXED-UHFFFAOYSA-N
Formula: C13H14O
SMILES: OC1(C#Cc2ccccc2)CCCC1
Mol. weight [g/mol]: 186.25
CAS: 25118-60-9

Physical Properties

Property code	Value	Unit	Source
gf	268.03	kJ/mol	Joback Method
hf	120.67	kJ/mol	Joback Method
hfus	18.31	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.343		Crippen Method
mcvol	156.680	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	640.22	K	Joback Method
tc	884.47	K	Joback Method
tf	464.41	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.04	J/mol×K	640.22	Joback Method
cpg	416.58	J/mol×K	680.93	Joback Method
cpg	431.13	J/mol×K	721.64	Joback Method
cpg	444.87	J/mol×K	762.35	Joback Method
cpg	458.02	J/mol×K	803.06	Joback Method
cpg	470.78	J/mol×K	843.77	Joback Method
cpg	483.33	J/mol×K	884.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25118609&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume