6-Phenyl-5-hexyn-3-ol

Inchi: InChI=1S/C12H14O/c1-2-12(13)10-6-9-11-7-4-3-5-8-11/h3-5,7-8,12-13H,2,10H2,1H3
InchiKey: JVUYLVMRBQNROA-UHFFFAOYSA-N
Formula: C12H14O
SMILES: CCC(O)CC#Cc1ccccc1
Mol. weight [g/mol]: 174.24
CAS: 135663-98-8

Physical Properties

Property code	Value	Unit	Source
gf	226.11	kJ/mol	Joback Method
hf	60.31	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.199		Crippen Method
mcvol	153.450	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	601.38	K	Joback Method
tc	814.92	K	Joback Method
tf	403.34	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.60	J/mol×K	601.38	Joback Method
cpg	381.02	J/mol×K	636.97	Joback Method
cpg	393.63	J/mol×K	672.56	Joback Method
cpg	405.45	J/mol×K	708.15	Joback Method
cpg	416.53	J/mol×K	743.74	Joback Method
cpg	426.91	J/mol×K	779.33	Joback Method
cpg	436.63	J/mol×K	814.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C135663988&Units=SI

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