1-Phenyl-1-octyne

Inchi: InChI=1S/C14H18/c1-2-3-4-5-6-8-11-14-12-9-7-10-13-14/h7,9-10,12-13H,2-6H2,1H3
InchiKey: YVCYLGYUDUYFQZ-UHFFFAOYSA-N
Formula: C14H18
SMILES: CCCCCCC#Cc1ccccc1
Mol. weight [g/mol]: 186.29
CAS: 16967-02-5

Physical Properties

Property code	Value	Unit	Source
gf	382.21	kJ/mol	Joback Method
hf	176.54	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.008		Crippen Method
mcvol	175.760	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
tb	555.40	K	Joback Method
tc	773.72	K	Joback Method
tf	380.06	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.20	J/mol×K	555.40	Joback Method
cpg	423.90	J/mol×K	591.79	Joback Method
cpg	440.56	J/mol×K	628.17	Joback Method
cpg	456.23	J/mol×K	664.56	Joback Method
cpg	470.95	J/mol×K	700.94	Joback Method
cpg	484.76	J/mol×K	737.33	Joback Method
cpg	497.72	J/mol×K	773.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16967025&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume