Benzene, 1-hexynyl-

Other names:	1-Hexyne, 1-phenyl-
	Butylphenylacetylene
	1-Butyl-2-phenylacetylene
	1-Phenyl-1-hexyne
	1-Hexynyl-benzene
Inchi:	InChI=1S/C12H14/c1-2-3-4-6-9-12-10-7-5-8-11-12/h5,7-8,10-11H,2-4H2,1H3
InchiKey:	VBRLZTLFLNZEPZ-UHFFFAOYSA-N
Formula:	C12H14
SMILES:	CCCCC#Cc1ccccc1
Mol. weight [g/mol]:	158.24
CAS:	1129-65-3

Physical Properties

Property code	Value	Unit	Source
gf	365.37	kJ/mol	Joback Method
hf	226.00	kJ/mol	NIST Webbook
hfus	24.00	kJ/mol	Joback Method
hvap	46.73	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.228		Crippen Method
mcvol	147.580	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	227.90		NIST Webbook
tb	503.50 ± 1.50	K	NIST Webbook
tb	503.70	K	NIST Webbook
tc	735.81	K	Joback Method
tf	357.52	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.48	J/mol×K	509.64	Joback Method
cpg	328.65	J/mol×K	547.34	Joback Method

cpg	343.83	J/mol×K	585.03	Joback Method
cpg	358.08	J/mol×K	622.73	Joback Method
cpg	371.43	J/mol×K	660.42	Joback Method
cpg	383.94	J/mol×K	698.12	Joback Method
cpg	395.64	J/mol×K	735.81	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=C1129653&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume