Benzene, 4-pentynyl-

Other names:	5-Phenyl-1-pentyne
	pent-4-ynylbenzene
Inchi:	InChI=1S/C11H12/c1-2-3-5-8-11-9-6-4-7-10-11/h1,4,6-7,9-10H,3,5,8H2
InchiKey:	KOSORCNALVBYBP-UHFFFAOYSA-N
Formula:	C11H12
SMILES:	C#CCCCc1ccccc1
Mol. weight [g/mol]:	144.21
CAS:	1823-14-9

Physical Properties

Property code	Value	Unit	Source
gf	377.22	kJ/mol	Joback Method
hf	258.06	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	42.21	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.643		Crippen Method
mcvol	133.490	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	467.88	K	Joback Method
tc	685.04	K	Joback Method
tf	287.12	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.66	J/mol×K	467.88	Joback Method
cpg	282.39	J/mol×K	504.07	Joback Method
cpg	296.20	J/mol×K	540.27	Joback Method
cpg	309.12	J/mol×K	576.46	Joback Method
cpg	321.21	J/mol×K	612.65	Joback Method
cpg	332.51	J/mol×K	648.85	Joback Method
cpg	343.07	J/mol×K	685.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1823149&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