Benzene, 1-methyl-4-(1-propynyl)-

Inchi: InChI=1S/C10H10/c1-3-4-10-7-5-9(2)6-8-10/h5-8H,1-2H3
InchiKey: NAYOGGQFBZAZIV-UHFFFAOYSA-N
Formula: C10H10
SMILES: CC#Cc1ccc(C)cc1
Mol. weight [g/mol]: 130.19
CAS: 2749-93-1

Physical Properties

Property code	Value	Unit	Source
gf	338.90	kJ/mol	Joback Method
hf	247.63	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	42.94	kJ/mol	Joback Method
ie	8.13 ± 0.02	eV	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.366		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
tb	468.86	K	Joback Method
tc	704.46	K	Joback Method
tf	347.50	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.63	J/mol×K	468.86	Joback Method
cpg	240.17	J/mol×K	508.13	Joback Method
cpg	252.92	J/mol×K	547.39	Joback Method
cpg	264.91	J/mol×K	586.66	Joback Method
cpg	276.15	J/mol×K	625.92	Joback Method
cpg	286.70	J/mol×K	665.19	Joback Method
cpg	296.57	J/mol×K	704.46	Joback Method

Sources

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=C2749931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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