4-Phenylbut-3-ene-1-yne

Other names: 1-Buten-3-yne, 1-phenyl
Inchi: InChI=1S/C10H8/c1-2-3-7-10-8-5-4-6-9-10/h1,3-9H/b7-3+
InchiKey: FRSPRPODGOIJPJ-XVNBXDOJSA-N
Formula: C10H8
SMILES: C#CC=Cc1ccccc1
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	449.02	kJ/mol	Joback Method
hf	395.92	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	39.95	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.333		Crippen Method
mcvol	115.100	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	190.30		NIST Webbook
tb	449.16	K	Joback Method
tc	681.13	K	Joback Method
tf	270.77	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.98	J/mol×K	449.16	Joback Method
cpg	223.16	J/mol×K	487.82	Joback Method
cpg	235.32	J/mol×K	526.48	Joback Method
cpg	246.53	J/mol×K	565.14	Joback Method
cpg	256.87	J/mol×K	603.81	Joback Method
cpg	266.39	J/mol×K	642.47	Joback Method
cpg	275.18	J/mol×K	681.13	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=U222120&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
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