1-Phenyl-1-pentyne

Other names: Benzene, 1-pentynyl-
1-pentynylbenzene
Inchi: InChI=1S/C11H12/c1-2-3-5-8-11-9-6-4-7-10-11/h4,6-7,9-10H,2-3H2,1H3
InchiKey: DEGIOKWPYFOHGH-UHFFFAOYSA-N
Formula: C11H12
SMILES: CCCC#Cc1ccccc1
Mol. weight [g/mol]: 144.21
CAS: 4250-81-1

Physical Properties

Property code	Value	Unit	Source
gf	356.95	kJ/mol	Joback Method
hf	238.46	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
ie	8.29 ± 0.02	eV	NIST Webbook
log10ws	-3.43		Crippen Method
logp	2.838		Crippen Method
mcvol	133.490	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	487.20	K	NIST Webbook
tb	486.00	K	NIST Webbook
tc	716.94	K	Joback Method
tf	346.25	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.36	J/mol×K	486.76	Joback Method
cpg	283.54	J/mol×K	525.12	Joback Method
cpg	297.79	J/mol×K	563.49	Joback Method
cpg	311.14	J/mol×K	601.85	Joback Method
cpg	323.64	J/mol×K	640.21	Joback Method

cpg	335.33	J/mol×K	678.58	Joback Method
cpg	346.26	J/mol×K	716.94	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.00	K	2.80	NIST Webbook

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=C4250811&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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