4-Phenyl-1-butyne

Other names: Benzene, 3-butynyl-
4-Phenyl-1-butyne
Inchi: InChI=1S/C10H10/c1-2-3-7-10-8-5-4-6-9-10/h1,4-6,8-9H,3,7H2
InchiKey: QDEOKXOYHYUKMS-UHFFFAOYSA-N
Formula: C10H10
SMILES: C#CCCc1ccccc1
Mol. weight [g/mol]: 130.19

Physical Properties

Property code	Value	Unit	Source
af	0.2931		Cheméo Relay (1.0)
chl	-5612.80	kJ/mol	NIST Webbook
gf	368.80	kJ/mol	Joback Method
hf	306.52	kJ/mol	Cheméo Relay (1.0)
hfl	248.60 ± 5.00	kJ/mol	NIST Webbook
hfl	-212.30	kJ/mol	NIST Webbook
hfus	18.67	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	NIST Webbook
log10ws	-2.82		Cheméo Relay (1.0)
logp	2.252		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1064.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
tb	463.00	K	NIST Webbook
tb	450.65 ± 3.00	K	NIST Webbook
tb	450.65 ± 3.00	K	NIST Webbook
tc	680.40	K	Cheméo Relay (1.0)
tf	225.87	K	Cheméo Relay (1.0)
vc	0.420	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.20	J/mol×K	445.00	Joback Method
cpg	239.84	J/mol×K	481.73	Joback Method
cpg	252.60	J/mol×K	518.45	Joback Method
cpg	264.52	J/mol×K	555.18	Joback Method
cpg	275.65	J/mol×K	591.91	Joback Method
cpg	286.02	J/mol×K	628.63	Joback Method
cpg	295.69	J/mol×K	665.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.00	K	0.50	NIST Webbook
tbrp	356.20	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16520620&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume