

3-Butynylbenzene

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
CAS:	16520-62-0

Physical Properties

Property code	Value	Unit	Source
chl	-5612.80	kJ/mol	NIST Webbook
gf	368.80	kJ/mol	Joback Method
hf	278.70	kJ/mol	Joback Method
hfl	-212.30	kJ/mol	NIST Webbook
hfl	248.60 ± 5.00	kJ/mol	NIST Webbook
hfus	18.67	kJ/mol	Joback Method
hvap	39.99	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.252		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1053.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1064.00		NIST Webbook
tb	450.65 ± 3.00	K	NIST Webbook
tb	463.00	K	NIST Webbook
tc	665.36	K	Joback Method
tf	275.85	K	Joback Method
vc	0.450	m3/kmol	Joback Method

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
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

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

Latest version available from:

<https://www.cheméo.com/cid/66-923-4/3-Butynylbenzene.pdf>

Generated by Cheméo on 2025-12-23 13:57:51.998283666 +0000 UTC m=+6246469.528324320.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.