1-Propyne, 3-bromo-

Other names:	Propyne, 3-bromo-
	Propargyl bromide
	1-Bromo-2-propyne
	2-Propynyl bromide
	3-Bromo-1-propyne
	3-Bromopropyne
	«gamma»-Bromoallylene
	1-Brom-2-propin
	UN 2345
	Progargyl bromide
	NSC 8801
Inchi:	InChI=1S/C3H3Br/c1-2-3-4/h1H,3H2
InchiKey:	YORCIIVHUBAYBQ-UHFFFAOYSA-N
Formula:	C3H3Br
SMILES:	C#CCBr
Mol. weight [g/mol]:	118.96
CAS:	106-96-7

Physical Properties

Property code	Value	Unit	Source
gf	211.77	kJ/mol	Joback Method
hf	212.98	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	28.56	kJ/mol	Joback Method
ie	10.47	eV	NIST Webbook
ie	10.48	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
log10ws	-1.30		Crippen Method
logp	1.014		Crippen Method
mcvol	62.030	ml/mol	McGowan Method
pc	6018.58	kPa	Joback Method
tb	362.20	K	NIST Webbook
tb	362.00 ± 1.00	K	NIST Webbook
tc	524.58	K	Joback Method
tf	230.34	K	Joback Method
vc	0.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	78.61	J/mol×K	324.32	Joback Method
cpg	82.58	J/mol×K	357.70	Joback Method
cpg	86.28	J/mol×K	391.07	Joback Method
cpg	89.71	J/mol×K	424.45	Joback Method
cpg	92.91	J/mol×K	457.83	Joback Method
cpg	95.88	J/mol×K	491.20	Joback Method
cpg	98.64	J/mol×K	524.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	306.20	K	17.30	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106967&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

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