

2-Butyne, 1,4-dichloro-

Other names:	1,4-Dichloro-2-butyne 1,4-Dichlorobutyne 1,4-dichlorobut-2-yne
Inchi:	InChI=1S/C4H4Cl2/c5-3-1-2-4-6/h3-4H2
InchiKey:	RCHDLEVSZBOHOS-UHFFFAOYSA-N
Formula:	C4H4Cl2
SMILES:	CICC#CCCI
Mol. weight [g/mol]:	122.98
CAS:	821-10-3

Physical Properties

Property code	Value	Unit	Source
gf	161.74	kJ/mol	Joback Method
hf	114.93	kJ/mol	Joback Method
hfus	17.63	kJ/mol	Joback Method
hvap	35.42	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.467		Crippen Method
mcvol	83.100	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
tb	438.70	K	NIST Webbook
tb	439.50 ± 1.50	K	NIST Webbook
tc	584.99	K	Joback Method
tf	300.78	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.13	J/molxK	374.78	Joback Method
cpg	122.43	J/molxK	409.82	Joback Method
cpg	127.48	J/molxK	444.85	Joback Method
cpg	132.29	J/molxK	479.89	Joback Method
cpg	136.87	J/molxK	514.92	Joback Method

cpg	141.23	J/mol×K	549.96	Joback Method
cpg	145.37	J/mol×K	584.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C821103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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