

Ethyne, dichloro-

Other names:	Acetylene, dichloro- Dichloroacetylene Dichloroethyne ClC«equiv»CCl C2Cl2
Inchi:	InChI=1S/C2Cl2/c3-1-2-4
InchiKey:	ZMJOVJSTYLQINE-UHFFFAOYSA-N
Formula:	C2Cl2
SMILES:	ClC#CCl
Mol. weight [g/mol]:	94.93
CAS:	7572-29-4

Physical Properties

Property code	Value	Unit	Source
gf	144.90	kJ/mol	Joback Method
hf	227.00 ± 14.00	kJ/mol	NIST Webbook
hfl	199.00 ± 14.00	kJ/mol	NIST Webbook
hfus	12.45	kJ/mol	Joback Method
hvap	27.40 ± 1.20	kJ/mol	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	9.90	eV	NIST Webbook
ie	10.03 ± 0.01	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
ie	10.30 ± 0.10	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
log10ws	-1.75		Crippen Method
logp	1.382		Crippen Method
mvol	54.920	ml/mol	McGowan Method
pc	5704.58	kPa	Joback Method
tb	329.02	K	Joback Method
tc	541.60	K	Joback Method
tf	147.15 ± 0.50	K	NIST Webbook
vc	0.207	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	60.06	J/mol×K	329.02	Joback Method
cpg	61.40	J/mol×K	364.45	Joback Method
cpg	62.67	J/mol×K	399.88	Joback Method
cpg	63.90	J/mol×K	435.31	Joback Method
cpg	65.06	J/mol×K	470.74	Joback Method
cpg	66.18	J/mol×K	506.17	Joback Method
cpg	67.25	J/mol×K	541.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7572294&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

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
mccvol:	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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