

1,4-Dichloro-1,3-butadiene

Inchi:	InChI=1S/C4H4Cl2/c5-3-1-2-4-6/h1-4H/b3-1+,4-2+
InchiKey:	LDZSRRMBFGBOAE-ZPUQHVIOSA-N
Formula:	C4H4Cl2
SMILES:	C1C=CC=CC1
Mol. weight [g/mol]:	122.98

Physical Properties

Property code	Value	Unit	Source
gf	119.38	kJ/mol	Joback Method
hf	77.07	kJ/mol	Joback Method
hfus	14.91	kJ/mol	Joback Method
hvap	33.18	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.491		Crippen Method
mcvol	83.100	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
rinpol	740.00		NIST Webbook
rinpol	740.00		NIST Webbook
tb	374.10	K	Joback Method
tc	576.61	K	Joback Method
tf	184.52	K	Joback Method
vc	0.318	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	111.82	J/molxK	374.10	Joback Method
cpg	139.46	J/molxK	542.86	Joback Method
cpg	134.80	J/molxK	509.11	Joback Method
cpg	129.73	J/molxK	475.36	Joback Method
cpg	124.24	J/molxK	441.60	Joback Method
cpg	118.28	J/molxK	407.85	Joback Method
cpg	143.76	J/molxK	576.61	Joback Method
dvisc	0.0002339	Paxs	374.10	Joback Method

dvisc	0.0002980	Paxs	342.50	Joback Method
dvisc	0.0003989	Paxs	310.91	Joback Method
dvisc	0.0005702	Paxs	279.31	Joback Method
dvisc	0.0008930	Paxs	247.71	Joback Method
dvisc	0.0015945	Paxs	216.12	Joback Method
dvisc	0.0034722	Paxs	184.52	Joback Method

Sources

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=R628045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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