cis-1,4-Dichloro-2-butene

Other names: 2-butene, 1,4-dichloro-, cis-
Inchi: InChI=1S/C4H6Cl2/c5-3-1-2-4-6/h1-2H,3-4H2/b2-1-
InchiKey: FQDIANVAWVHZIR-UPHRSURJSA-N
Formula: C4H6Cl2
SMILES: ClCC=CCCl
Mol. weight [g/mol]: 125.00

Physical Properties

Property code	Value	Unit	Source
gf	39.16	kJ/mol	Joback Method
hf	-40.15	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	33.23	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	2.020		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	3791.65	kPa	Joback Method
rinpol	874.00		NIST Webbook
tb	369.94	K	Joback Method
tc	561.81	K	Joback Method
tf	189.60	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.84	J/mol×K	369.94	Joback Method
cpg	133.79	J/mol×K	401.92	Joback Method
cpg	140.33	J/mol×K	433.90	Joback Method
cpg	146.50	J/mol×K	465.87	Joback Method
cpg	152.30	J/mol×K	497.85	Joback Method
cpg	157.76	J/mol×K	529.83	Joback Method
cpg	162.91	J/mol×K	561.81	Joback Method
dvisc	0.0037801	Pa×s	189.60	Joback Method

dvisc	0.0018290	Pa×s	219.66	Joback Method
dvisc	0.0010539	Pa×s	249.71	Joback Method
dvisc	0.0006837	Pa×s	279.77	Joback Method
dvisc	0.0004823	Pa×s	309.83	Joback Method
dvisc	0.0003620	Pa×s	339.88	Joback Method
dvisc	0.0002846	Pa×s	369.94	Joback Method

Sources

Determination of Henry's Law Constants Using Internal Standards with Benchmark Values:	https://www.doi.org/10.1021/je3010535
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=R596359&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