3,3-Dichloro-2-propene-1-ol

Inchi: InChI=1S/C3H4Cl2O/c4-3(5)1-2-6/h1,6H,2H2
InchiKey: KJEGVVJINLACNZ-UHFFFAOYSA-N
Formula: C3H4Cl2O
SMILES: OCC=C(Cl)Cl
Mol. weight [g/mol]: 126.97
CAS: 3039-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-114.63	kJ/mol	Joback Method
hf	-181.53	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	47.76	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.298		Crippen Method
mcvol	79.180	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	439.12	K	Joback Method
tc	628.63	K	Joback Method
tf	225.19	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.20	J/mol×K	439.12	Joback Method
cpg	129.92	J/mol×K	470.70	Joback Method
cpg	134.33	J/mol×K	502.29	Joback Method
cpg	138.46	J/mol×K	533.87	Joback Method
cpg	142.32	J/mol×K	565.46	Joback Method
cpg	145.93	J/mol×K	597.04	Joback Method
cpg	149.31	J/mol×K	628.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3039552&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume