3-Chloro-2-buten-1-ol

Other names: 2-Buten-1-ol, 3-chloro-
3-Chloro-2-butene-1-ol
Inchi: InChI=1S/C4H7ClO/c1-4(5)2-3-6/h2,6H,3H2,1H3/b4-2-
InchiKey: SRQGZQPUPABHCN-RQOWECAXSA-N
Formula: C4H7ClO
SMILES: CC(Cl)=CCO
Mol. weight [g/mol]: 106.55
CAS: 40605-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-94.28	kJ/mol	Joback Method
hf	-186.43	kJ/mol	Joback Method
hfus	13.29	kJ/mol	Joback Method
hvap	45.60	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	1.121		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	424.57	K	Joback Method
tc	605.66	K	Joback Method
tf	206.54	K	Joback Method
vc	0.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.67	J/mol×K	424.57	Joback Method
cpg	147.14	J/mol×K	454.75	Joback Method
cpg	153.26	J/mol×K	484.93	Joback Method
cpg	159.06	J/mol×K	515.12	Joback Method
cpg	164.55	J/mol×K	545.30	Joback Method
cpg	169.75	J/mol×K	575.48	Joback Method
cpg	174.68	J/mol×K	605.66	Joback Method

hvapt	50.00	kJ/mol	391.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.27947e+01
Coeff. B	-5.12204e+03
Coeff. C	-1.09720e+02
Temperature range (K), min.	337.29
Temperature range (K), max.	402.69

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40605423&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure

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