Oxetane, 3-chloromethyl-3-hydroxymethyl

Inchi: InChI=1S/C5H9ClO2/c6-1-5(2-7)3-8-4-5/h7H,1-4H2
InchiKey: BIZNEDGOZPNEPL-UHFFFAOYSA-N
Formula: C5H9ClO2
SMILES: OCC1(CCl)COC1
Mol. weight [g/mol]: 136.58

Physical Properties

Property code	Value	Unit	Source
gf	-200.49	kJ/mol	Joback Method
hf	-364.62	kJ/mol	Joback Method
hfus	14.71	kJ/mol	Joback Method
hvap	51.23	kJ/mol	Joback Method
log10ws	-0.07		Crippen Method
logp	0.234		Crippen Method
mcvol	94.430	ml/mol	McGowan Method
pc	4743.15	kPa	Joback Method
rinpol	1142.00		NIST Webbook
tb	481.61	K	Joback Method
tc	677.88	K	Joback Method
tf	301.74	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.51	J/mol×K	481.61	Joback Method
cpg	212.65	J/mol×K	514.32	Joback Method
cpg	221.06	J/mol×K	547.03	Joback Method
cpg	228.86	J/mol×K	579.74	Joback Method
cpg	236.11	J/mol×K	612.46	Joback Method
cpg	242.92	J/mol×K	645.17	Joback Method
cpg	249.36	J/mol×K	677.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6683&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume