Oxetane, 3-chloromethyl-3-iodomethyl

Inchi: InChI=1S/C5H8ClIO/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: AAHVBCSCIJYASL-UHFFFAOYSA-N
Formula: C5H8ClIO
SMILES: ClCC1(CI)COC1
Mol. weight [g/mol]: 246.47

Physical Properties

Property code	Value	Unit	Source
gf	-5.55	kJ/mol	Joback Method
hf	-135.52	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	43.93	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.677		Crippen Method
mcvol	114.380	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
rinpol	1249.00		NIST Webbook
tb	482.57	K	Joback Method
tc	728.91	K	Joback Method
tf	298.98	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.11	J/mol×K	482.57	Joback Method
cpg	214.47	J/mol×K	523.63	Joback Method
cpg	223.72	J/mol×K	564.68	Joback Method
cpg	232.07	J/mol×K	605.74	Joback Method
cpg	239.69	J/mol×K	646.80	Joback Method
cpg	246.78	J/mol×K	687.85	Joback Method
cpg	253.52	J/mol×K	728.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6696&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