Oxetane, 3-hydroxymethyl-3-iodomethyl

Inchi: InChI=1S/C5H9IO2/c6-1-5(2-7)3-8-4-5/h7H,1-4H2
InchiKey: KFKOWZQKJBZPTJ-UHFFFAOYSA-N
Formula: C5H9IO2
SMILES: OCC1(CI)COC1
Mol. weight [g/mol]: 228.03

Physical Properties

Property code	Value	Unit	Source
gf	-130.44	kJ/mol	Joback Method
hf	-272.01	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	56.22	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.430		Crippen Method
mcvol	108.010	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
rinpol	1309.00		NIST Webbook
tb	537.32	K	Joback Method
tc	758.89	K	Joback Method
tf	329.88	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.92	J/mol×K	537.32	Joback Method
cpg	230.61	J/mol×K	574.25	Joback Method
cpg	238.58	J/mol×K	611.18	Joback Method
cpg	245.97	J/mol×K	648.10	Joback Method
cpg	252.90	J/mol×K	685.03	Joback Method
cpg	259.52	J/mol×K	721.96	Joback Method
cpg	265.97	J/mol×K	758.89	Joback Method

Sources

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=R6756&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
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