Oxetane, 3-diiodomethyl

Inchi: InChI=1S/C5H8I2O/c6-1-5(2-7)3-8-4-5/h1-4H2
InchiKey: JRMFTYIUHNPQQY-UHFFFAOYSA-N
Formula: C5H8I2O
SMILES: ICC1(CI)COC1
Mol. weight [g/mol]: 337.93

Physical Properties

Property code	Value	Unit	Source
gf	64.50	kJ/mol	Joback Method
hf	-42.91	kJ/mol	Joback Method
hfus	15.23	kJ/mol	Joback Method
hvap	48.91	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.873		Crippen Method
mcvol	127.960	ml/mol	McGowan Method
pc	4156.97	kPa	Joback Method
rinpol	1412.00		NIST Webbook
rinpol	1412.00		NIST Webbook
tb	538.28	K	Joback Method
tc	816.67	K	Joback Method
tf	327.12	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.16	J/mol×K	538.28	Joback Method
cpg	230.84	J/mol×K	584.68	Joback Method
cpg	239.44	J/mol×K	631.08	Joback Method
cpg	247.25	J/mol×K	677.47	Joback Method
cpg	254.57	J/mol×K	723.87	Joback Method
cpg	261.70	J/mol×K	770.27	Joback Method
cpg	268.91	J/mol×K	816.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6701&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