2,3,3-Trimethyl-oxetane

Inchi: InChI=1S/C6H12O/c1-5-6(2,3)4-7-5/h5H,4H2,1-3H3
InchiKey: KUTQUJKLMUSJFL-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC1OCC1(C)C
Mol. weight [g/mol]: 100.16

Physical Properties

Property code	Value	Unit	Source
gf	-51.03	kJ/mol	Joback Method
hf	-237.63	kJ/mol	Joback Method
hfus	10.08	kJ/mol	Joback Method
hvap	32.09	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	715.00		NIST Webbook
tb	370.21	K	Joback Method
tc	566.43	K	Joback Method
tf	218.03	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.28	J/mol×K	370.21	Joback Method
cpg	182.22	J/mol×K	402.91	Joback Method
cpg	195.16	J/mol×K	435.62	Joback Method
cpg	207.18	J/mol×K	468.32	Joback Method
cpg	218.37	J/mol×K	501.02	Joback Method
cpg	228.80	J/mol×K	533.72	Joback Method
cpg	238.57	J/mol×K	566.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405684&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

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