Oxetane, 3-methyl-3-(1-methylethyl)

Inchi: InChI=1S/C7H14O/c1-6(2)7(3)4-8-5-7/h6H,4-5H2,1-3H3
InchiKey: DESPTAAIBOOLQX-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CC(C)C1(C)COC1
Mol. weight [g/mol]: 114.19

Physical Properties

Property code	Value	Unit	Source
gf	-37.34	kJ/mol	Joback Method
hf	-243.21	kJ/mol	Joback Method
hfus	8.08	kJ/mol	Joback Method
hvap	34.23	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.679		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	850.00		NIST Webbook
tb	397.32	K	Joback Method
tc	597.60	K	Joback Method
tf	218.54	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.64	J/mol×K	397.32	Joback Method
cpg	221.82	J/mol×K	430.70	Joback Method
cpg	235.89	J/mol×K	464.08	Joback Method
cpg	248.95	J/mol×K	497.46	Joback Method
cpg	261.09	J/mol×K	530.84	Joback Method
cpg	272.42	J/mol×K	564.22	Joback Method
cpg	283.02	J/mol×K	597.60	Joback Method

Sources

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=R6798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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