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

Inchi: InChI=1S/C8H16O/c1-7(2,3)8(4)5-9-6-8/h5-6H2,1-4H3
InchiKey: ALEYSGNQEYIRHZ-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CC(C)(C)C1(C)COC1
Mol. weight [g/mol]: 128.21

Physical Properties

Property code	Value	Unit	Source
gf	-23.64	kJ/mol	Joback Method
hf	-267.32	kJ/mol	Joback Method
hfus	6.78	kJ/mol	Joback Method
hvap	35.55	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	2.069		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	924.00		NIST Webbook
tb	417.41	K	Joback Method
tc	624.61	K	Joback Method
tf	247.23	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.20	J/mol×K	417.41	Joback Method
cpg	266.56	J/mol×K	451.94	Joback Method
cpg	282.54	J/mol×K	486.48	Joback Method
cpg	297.27	J/mol×K	521.01	Joback Method
cpg	310.87	J/mol×K	555.54	Joback Method
cpg	323.48	J/mol×K	590.08	Joback Method
cpg	335.22	J/mol×K	624.61	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=R6785&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