Oxetane, 3-methyl

Other names: 3-Methyl-oxetane
Inchi: InChI=1S/C4H8O/c1-4-2-5-3-4/h4H,2-3H2,1H3
InchiKey: VJQHJNIGWOABDZ-UHFFFAOYSA-N
Formula: C4H8O
SMILES: CC1COC1
Mol. weight [g/mol]: 72.11

Physical Properties

Property code	Value	Unit	Source
gf	-54.67	kJ/mol	Joback Method
hf	-191.25	kJ/mol	Joback Method
hfus	10.13	kJ/mol	Joback Method
hvap	29.09	kJ/mol	Joback Method
log10ws	-0.24		Crippen Method
logp	0.653		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	583.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	583.00		NIST Webbook
tb	328.88	K	Joback Method
tc	517.93	K	Joback Method
tf	175.83	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	98.12	J/mol×K	328.88	Joback Method
cpg	142.67	J/mol×K	486.42	Joback Method
cpg	134.67	J/mol×K	454.91	Joback Method
cpg	126.24	J/mol×K	423.40	Joback Method
cpg	117.35	J/mol×K	391.90	Joback Method
cpg	107.98	J/mol×K	360.39	Joback Method

cpg	150.24	J/mol×K	517.93	Joback Method
dvisc	0.0003092	Pa×s	328.88	Joback Method
dvisc	0.0003615	Pa×s	303.37	Joback Method
dvisc	0.0004350	Pa×s	277.86	Joback Method
dvisc	0.0005434	Pa×s	252.35	Joback Method
dvisc	0.0007135	Pa×s	226.85	Joback Method
dvisc	0.0010040	Pa×s	201.34	Joback Method
dvisc	0.0015598	Pa×s	175.83	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R6772&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
dvisc: Dynamic viscosity
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

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