

3-Methyl-3-oxetanemethanol

Other names:	Oxetane, 3-hydroxymethyl-3-methyl
Inchi:	InChI=1S/C5H10O2/c1-5(2-6)3-7-4-5/h6H,2-4H2,1H3
InchiKey:	NLQMSBJFLQPLIJ-UHFFFAOYSA-N
Formula:	C5H10O2
SMILES:	CC1(CO)COC1
Mol. weight [g/mol]:	102.13
CAS:	3143-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-188.56	kJ/mol	Joback Method
hf	-348.88	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	46.85	kJ/mol	Joback Method
log10ws	0.08		Crippen Method
logp	0.015		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
rinpol	920.00		NIST Webbook
tb	444.18	K	Joback Method
tc	634.31	K	Joback Method
tf	271.82	K	Joback Method
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.40	J/mol×K	444.18	Joback Method
cpg	189.36	J/mol×K	475.87	Joback Method
cpg	198.57	J/mol×K	507.56	Joback Method
cpg	207.09	J/mol×K	539.25	Joback Method
cpg	215.03	J/mol×K	570.94	Joback Method
cpg	222.44	J/mol×K	602.63	Joback Method
cpg	229.42	J/mol×K	634.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.20	K	5.30	NIST Webbook
tbrp	353.00	K	5.30	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3143020&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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