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

Physical Properties

Property code	Value	Unit	Source
hf	-326.99	kJ/mol	Cheméo Relay (1.0)
hfus	10.51	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Cheméo Relay (1.0)
logp	0.015		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
rinpol	920.00		NIST Webbook
tb	438.10	K	Cheméo Relay (1.0)
tf	356.21	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3143020&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point