2-Methyl-oxetane

Other names: 2-Methyl-oxetane
Inchi: InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3
InchiKey: FZIIBDOXPQOKBP-UHFFFAOYSA-N
Formula: C4H8O
SMILES: CC1CCO1
Mol. weight [g/mol]: 72.11

Physical Properties

Property code	Value	Unit	Source
af	0.2549		Cheméo Relay (1.0)
gf	-54.67	kJ/mol	Joback Method
hf	-156.39	kJ/mol	Cheméo Relay (1.0)
hfus	10.13	kJ/mol	Joback Method
hvap	28.31	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	0.24		Cheméo Relay (1.0)
logp	0.795		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	543.00		NIST Webbook
rinpol	572.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	573.00		NIST Webbook
tb	318.89	K	Cheméo Relay (1.0)
tc	492.75	K	Cheméo Relay (1.0)
tf	147.07	K	Cheméo Relay (1.0)
vc	0.227	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	98.12	J/mol×K	328.88	Joback Method
cpg	107.98	J/mol×K	360.39	Joback Method

cpg	117.35	J/mol×K	391.90	Joback Method
cpg	126.24	J/mol×K	423.40	Joback Method
cpg	134.67	J/mol×K	454.91	Joback Method
cpg	142.67	J/mol×K	486.42	Joback Method
cpg	150.24	J/mol×K	517.93	Joback Method
dvisc	0.0015598	Pa×s	175.83	Joback Method
dvisc	0.0010040	Pa×s	201.34	Joback Method
dvisc	0.0007135	Pa×s	226.85	Joback Method
dvisc	0.0005434	Pa×s	252.35	Joback Method
dvisc	0.0004350	Pa×s	277.86	Joback Method
dvisc	0.0003615	Pa×s	303.37	Joback Method
dvisc	0.0003092	Pa×s	328.88	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2167397&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor
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
ie: Ionization energy
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