

Oxetane, 2-methyl-

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
CAS:	2167-39-7

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	-0.59		Crippen Method
logp	0.795		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	572.00		NIST Webbook
rinpol	573.00		NIST Webbook
rinpol	578.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	578.00		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/molxK	328.88	Joback Method
cpg	107.98	J/molxK	360.39	Joback Method
cpg	117.35	J/molxK	391.90	Joback Method

cpg	126.24	J/molxK	423.40	Joback Method
cpg	134.67	J/molxK	454.91	Joback Method
cpg	142.67	J/molxK	486.42	Joback Method
cpg	150.24	J/molxK	517.93	Joback Method
dvisc	0.0015598	Paxs	175.83	Joback Method
dvisc	0.0010040	Paxs	201.34	Joback Method
dvisc	0.0007135	Paxs	226.85	Joback Method
dvisc	0.0005434	Paxs	252.35	Joback Method
dvisc	0.0004350	Paxs	277.86	Joback Method
dvisc	0.0003615	Paxs	303.37	Joback Method
dvisc	0.0003092	Paxs	328.88	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=C2167397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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