

Oxetane, 3-methylene

Inchi: InChI=1S/C4H6O/c1-4-2-5-3-4/h1-3H2
InchiKey: FONJUXZYNZCFSE-UHFFFAOYSA-N
Formula: C4H6O
SMILES: C=C1COC1
Mol. weight [g/mol]: 70.09

Physical Properties

Property code	Value	Unit	Source
gf	6.12	kJ/mol	Joback Method
hf	-86.67	kJ/mol	Joback Method
hfus	7.90	kJ/mol	Joback Method
hvap	29.56	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.573		Crippen Method
mcvol	57.930	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
rinpol	574.00		NIST Webbook
tb	332.71	K	Joback Method
tc	524.46	K	Joback Method
tf	193.75	K	Joback Method
vc	0.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	89.48	J/mol×K	332.71	Joback Method
cpg	124.55	J/mol×K	492.50	Joback Method
cpg	118.32	J/mol×K	460.54	Joback Method
cpg	111.72	J/mol×K	428.58	Joback Method
cpg	104.73	J/mol×K	396.63	Joback Method
cpg	97.32	J/mol×K	364.67	Joback Method
cpg	130.42	J/mol×K	524.46	Joback Method
dvisc	0.0003341	Pa×s	332.71	Joback Method
dvisc	0.0003917	Pa×s	309.55	Joback Method

dvisc	0.0004711	Pa×s	286.39	Joback Method
dvisc	0.0005854	Pa×s	263.23	Joback Method
dvisc	0.0007584	Pa×s	240.07	Joback Method
dvisc	0.0010385	Pa×s	216.91	Joback Method
dvisc	0.0015331	Pa×s	193.75	Joback Method

Sources

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=R127438&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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