Oxetane, 3,3-diethyl

Inchi: InChI=1S/C7H14O/c1-3-7(4-2)5-8-6-7/h3-6H2,1-2H3
InchiKey: VFYHHERJNPKXIX-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CCC1(CC)COC1
Mol. weight [g/mol]: 114.19
CAS: 10196-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-34.90	kJ/mol	Joback Method
hf	-237.93	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	34.62	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.823		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	888.00		NIST Webbook
rinpol	888.00		NIST Webbook
tb	397.76	K	Joback Method
tc	593.23	K	Joback Method
tf	233.54	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.71	J/mol×K	397.76	Joback Method
cpg	221.43	J/mol×K	430.34	Joback Method
cpg	235.09	J/mol×K	462.92	Joback Method
cpg	247.80	J/mol×K	495.49	Joback Method
cpg	259.64	J/mol×K	528.07	Joback Method
cpg	270.70	J/mol×K	560.65	Joback Method
cpg	281.07	J/mol×K	593.23	Joback Method

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=C10196391&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume