Oxetane, 3-ethyl-3-methyl

Inchi: InChI=1S/C6H12O/c1-3-6(2)4-7-5-6/h3-5H2,1-2H3
InchiKey: LXGCIBZDAQMLHO-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CCC1(C)COC1
Mol. weight [g/mol]: 100.16
CAS: 35737-67-8

Physical Properties

Property code	Value	Unit	Source
gf	-43.32	kJ/mol	Joback Method
hf	-217.29	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	32.39	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	1.433		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
rinpol	774.00		NIST Webbook
rinpol	774.00		NIST Webbook
tb	374.88	K	Joback Method
tc	571.74	K	Joback Method
tf	222.27	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.02	J/mol×K	374.88	Joback Method
cpg	181.73	J/mol×K	407.69	Joback Method
cpg	194.40	J/mol×K	440.50	Joback Method
cpg	206.12	J/mol×K	473.31	Joback Method
cpg	216.97	J/mol×K	506.12	Joback Method
cpg	227.06	J/mol×K	538.93	Joback Method
cpg	236.46	J/mol×K	571.74	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=C35737678&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