Oxetane, 3-ethyl-3-(3-methylbutyl)

Inchi: InChI=1S/C10H20O/c1-4-10(7-11-8-10)6-5-9(2)3/h9H,4-8H2,1-3H3
InchiKey: WMKRRKIKWFHFAQ-UHFFFAOYSA-N
Formula: C10H20O
SMILES: CCC1(CCC(C)C)COC1
Mol. weight [g/mol]: 156.27

Physical Properties

Property code	Value	Unit	Source
gf	-12.08	kJ/mol	Joback Method
hf	-305.13	kJ/mol	Joback Method
hfus	15.85	kJ/mol	Joback Method
hvap	40.91	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.849		Crippen Method
mcvol	146.770	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	465.96	K	Joback Method
tc	660.14	K	Joback Method
tf	252.35	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.90	J/mol×K	465.96	Joback Method
cpg	352.46	J/mol×K	498.32	Joback Method
cpg	368.93	J/mol×K	530.69	Joback Method
cpg	384.41	J/mol×K	563.05	Joback Method
cpg	398.99	J/mol×K	595.41	Joback Method
cpg	412.77	J/mol×K	627.78	Joback Method
cpg	425.84	J/mol×K	660.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R6727&Units=SI
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

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