Oxetane, 3-ethyl-3-butyl

Inchi: InChI=1S/C9H18O/c1-3-5-6-9(4-2)7-10-8-9/h3-8H2,1-2H3
InchiKey: CENXSGFRWSXCQU-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCCC1(CC)COC1
Mol. weight [g/mol]: 142.24

Physical Properties

Property code	Value	Unit	Source
gf	-18.06	kJ/mol	Joback Method
hf	-279.21	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	39.07	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.603		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1075.00		NIST Webbook
tb	443.52	K	Joback Method
tc	635.43	K	Joback Method
tf	256.08	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.20	J/mol×K	443.52	Joback Method
cpg	306.60	J/mol×K	475.50	Joback Method
cpg	321.95	J/mol×K	507.49	Joback Method
cpg	336.35	J/mol×K	539.47	Joback Method
cpg	349.88	J/mol×K	571.46	Joback Method
cpg	362.64	J/mol×K	603.44	Joback Method
cpg	374.72	J/mol×K	635.43	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=R6730&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