Oxetane, 3-ethyl-3-propyl

Inchi: InChI=1S/C8H16O/c1-3-5-8(4-2)6-9-7-8/h3-7H2,1-2H3
InchiKey: HAJCTSOSULRGRA-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC1(CC)COC1
Mol. weight [g/mol]: 128.21

Physical Properties

Property code	Value	Unit	Source
gf	-26.48	kJ/mol	Joback Method
hf	-258.57	kJ/mol	Joback Method
hfus	14.19	kJ/mol	Joback Method
hvap	36.85	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	2.213		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	987.00		NIST Webbook
tb	420.64	K	Joback Method
tc	614.43	K	Joback Method
tf	244.81	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.47	J/mol×K	420.64	Joback Method
cpg	263.08	J/mol×K	452.94	Joback Method
cpg	277.64	J/mol×K	485.24	Joback Method
cpg	291.24	J/mol×K	517.54	Joback Method
cpg	303.97	J/mol×K	549.83	Joback Method
cpg	315.92	J/mol×K	582.13	Joback Method
cpg	327.18	J/mol×K	614.43	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=R6743&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
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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