Oxirane, 3-ethyl-2,2-dimethyl-

Other names:	Pentane, 2,3-epoxy-2-methyl-
	2-Methyl-2-pentene oxide
	2,3-Epoxy-2-methylpentane
	2-Methyl-2,3-pentylene oxide
	2-Methyl-2,3-epoxypentane
	3-Ethyl-2,2-dimethyl oxirane
Inchi:	InChI=1S/C6H12O/c1-4-5-6(2,3)7-5/h5H,4H2,1-3H3
InchiKey:	OZVWXRGXOYUQEJ-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCC1OC1(C)C
Mol. weight [g/mol]:	100.16
CAS:	1192-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-38.93	kJ/mol	Joback Method
hf	-231.47	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	31.91	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.574		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	700.60		NIST Webbook
rinpol	700.30		NIST Webbook
rinpol	701.40		NIST Webbook
rinpol	701.40		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	700.30		NIST Webbook
tb	365.94	K	Joback Method
tc	553.87	K	Joback Method
tf	221.55	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.26	J/mol×K	365.94	Joback Method
cpg	183.37	J/mol×K	397.26	Joback Method
cpg	195.52	J/mol×K	428.58	Joback Method
cpg	206.80	J/mol×K	459.90	Joback Method
cpg	217.29	J/mol×K	491.22	Joback Method
cpg	227.05	J/mol×K	522.54	Joback Method
cpg	236.18	J/mol×K	553.87	Joback Method
hvapt	40.60	kJ/mol	337.50	NIST Webbook

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=C1192229&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
hvapt: Enthalpy of vaporization at a given temperature
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