2-Ethyl-2,3-dimethyl-oxirane (E)

Inchi: InChI=1S/C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3
InchiKey: ZISUZIXPPXXNPC-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CCC1(C)OC1C
Mol. weight [g/mol]: 100.16

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	720.00		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

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=R405728&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

Latest version available from:
https://www.chemeo.com/cid/34-328-0/2-Ethyl-2-3-dimethyl-oxirane-E.pdf
Generated by Cheméo on 2024-10-12 07:35:28.083228941 +0000 UTC m=+3299390.720198199.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.