Oxirane, 2-ethyl-2-methyl-

Other names: Butane, 1,2-epoxy-2-methyl-
2-Ethyl-2-methyloxirane
2-Methyl-1-butene oxide
1,2-Epoxy-2-methylbutane
Inchi: InChI=1S/C5H10O/c1-3-5(2)4-6-5/h3-4H2,1-2H3
InchiKey: QZXUQPKFNQQQAJ-UHFFFAOYSA-N
Formula: C5H10O
SMILES: CCC1(C)CO1
Mol. weight [g/mol]: 86.13
CAS: 30095-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-39.64	kJ/mol	Joback Method
hf	-190.49	kJ/mol	Joback Method
hfus	8.52	kJ/mol	Joback Method
hvap	30.00	kJ/mol	Joback Method
log10ws	-1.01		Crippen Method
logp	1.185		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
rinpol	634.00		NIST Webbook
rinpol	633.70		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	633.30		NIST Webbook
rinpol	634.00		NIST Webbook
rinpol	634.00		NIST Webbook
tb	354.65 ± 3.00	K	NIST Webbook
tc	536.99	K	Joback Method
tf	214.52	K	Joback Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.88	J/mol×K	347.73	Joback Method
cpg	145.69	J/mol×K	379.27	Joback Method
cpg	156.52	J/mol×K	410.82	Joback Method
cpg	166.46	J/mol×K	442.36	Joback Method
cpg	175.59	J/mol×K	473.90	Joback Method
cpg	183.99	J/mol×K	505.45	Joback Method
cpg	191.74	J/mol×K	536.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30095637&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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