2,2-Diethyl-oxirane

Other names: oxirane, 1,1-diethyl-
Inchi: InChI=1S/C6H12O/c1-3-6(4-2)5-7-6/h3-5H2,1-2H3
InchiKey: OVKYVUFYOFPYNK-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CCC1(CC)CO1
Mol. weight [g/mol]: 100.16
CAS: 1192-17-2

Physical Properties

Property code	Value	Unit	Source
gf	-31.22	kJ/mol	Joback Method
hf	-211.13	kJ/mol	Joback Method
hfus	11.11	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.575		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	542.00		NIST Webbook
tb	378.65 ± 2.00	K	NIST Webbook
tc	559.20	K	Joback Method
tf	225.79	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.98	J/mol×K	370.61	Joback Method
cpg	182.87	J/mol×K	402.04	Joback Method
cpg	194.77	J/mol×K	433.47	Joback Method
cpg	205.76	J/mol×K	464.91	Joback Method
cpg	215.93	J/mol×K	496.34	Joback Method
cpg	225.37	J/mol×K	527.77	Joback Method
cpg	234.15	J/mol×K	559.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192172&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