3,3-Dimethyl-1,2-epoxybutane

Other names:	Oxirane, (1,1-dimethylethyl)- tert-Butylethylene oxide tert-Butyloxirane Butane, 1,2-epoxy-3,3-dimethyl- 2-tert-Butyloxirane 3,3-Dimethylbutene oxide Oxirane, 2-(1,1-dimethylethyl)- 1,1-Dimethylethyl-oxirane
Inchi:	InChI=1S/C6H12O/c1-6(2,3)5-4-7-5/h5H,4H2,1-3H3
InchiKey:	HEAYDCIZOFDHRM-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(C)(C)C1CO1
Mol. weight [g/mol]:	100.16
CAS:	2245-30-9

Physical Properties

Property code	Value	Unit	Source
gf	-22.89	kJ/mol	Joback Method
hf	-235.12	kJ/mol	Joback Method
hfus	10.00	kJ/mol	Joback Method
hvap	32.08	kJ/mol	Joback Method
ie	10.04 ± 0.05	eV	NIST Webbook
log10ws	-1.19		Crippen Method
logp	1.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	705.00		NIST Webbook
rinpol	705.00		NIST Webbook
tb	379.15 ± 3.00	K	NIST Webbook
tb	380.15 ± 2.00	K	NIST Webbook
tb	374.47 ± 0.50	K	NIST Webbook
tc	560.00	K	Joback Method
tf	204.31	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.48	J/mol×K	367.14	Joback Method
cpg	184.11	J/mol×K	399.28	Joback Method
cpg	196.89	J/mol×K	431.43	Joback Method
cpg	208.85	J/mol×K	463.57	Joback Method
cpg	220.05	J/mol×K	495.72	Joback Method
cpg	230.52	J/mol×K	527.86	Joback Method
cpg	240.32	J/mol×K	560.00	Joback Method
dvisc	0.0027460	Pa×s	204.31	Joback Method
dvisc	0.0017084	Pa×s	231.45	Joback Method
dvisc	0.0011742	Pa×s	258.59	Joback Method
dvisc	0.0008666	Pa×s	285.73	Joback Method
dvisc	0.0006742	Pa×s	312.86	Joback Method
dvisc	0.0005460	Pa×s	340.00	Joback Method
dvisc	0.0004561	Pa×s	367.14	Joback Method

Sources

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=C2245309&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ie: Ionization energy
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