Oxirane, 2-methyl-2-(1-methylethyl)-

Other names:	2,3-dimethyl-1,2-epoxybutane
	2-Methyl-2-(1-methylethyl)-oxirane
	2-isopropyl-2-methyloxirane
Inchi:	InChI=1S/C6H12O/c1-5(2)6(3)4-7-6/h5H,4H2,1-3H3
InchiKey:	JATXAMXFNMUGBL-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(C)C1(C)CO1
Mol. weight [g/mol]:	100.16
CAS:	72221-03-5

Physical Properties

Property code	Value	Unit	Source
gf	-33.66	kJ/mol	Joback Method
hf	-216.41	kJ/mol	Joback Method
hfus	7.59	kJ/mol	Joback Method
hvap	31.83	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3810.39	kPa	Joback Method
rinpol	718.40		NIST Webbook
rinpol	718.40		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	712.00		NIST Webbook
rinpol	717.50		NIST Webbook
rinpol	716.90		NIST Webbook
tb	370.17	K	Joback Method
tc	563.45	K	Joback Method
tf	210.79	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	169.84	J/mol×K	370.17	Joback Method
cpg	183.15	J/mol×K	402.38	Joback Method
cpg	195.42	J/mol×K	434.60	Joback Method
cpg	206.73	J/mol×K	466.81	Joback Method
cpg	217.18	J/mol×K	499.03	Joback Method
cpg	226.85	J/mol×K	531.24	Joback Method
cpg	235.84	J/mol×K	563.45	Joback Method

Sources

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=C72221035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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