Oxirane, (2-methylpropyl)-

Other names:	Pentane, 1,2-epoxy-4-methyl-
	1,2-Epoxy-4-methylpentane
	2-Isobutyloxirane
	4-Methyl-1,2-epoxypentane
	Isobutyloxirane
Inchi:	InChI=1S/C6H12O/c1-5(2)3-6-4-7-6/h5-6H,3-4H2,1-2H3
InchiKey:	YXIOECOAAMLHPG-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(C)CC1CO1
Mol. weight [g/mol]:	100.16
CAS:	23850-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-28.17	kJ/mol	Joback Method
hf	-231.65	kJ/mol	Joback Method
hfus	13.89	kJ/mol	Joback Method
hvap	32.98	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
rinpol	721.00		NIST Webbook
rinpol	751.20		NIST Webbook
rinpol	751.80		NIST Webbook
rinpol	753.40		NIST Webbook
rinpol	753.40		NIST Webbook
rinpol	721.00		NIST Webbook
tb	369.93	K	Joback Method
tc	554.59	K	Joback Method
tf	186.89	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.54	J/mol×K	369.93	Joback Method
cpg	225.07	J/mol×K	523.81	Joback Method
cpg	215.11	J/mol×K	493.03	Joback Method
cpg	204.61	J/mol×K	462.26	Joback Method
cpg	193.53	J/mol×K	431.48	Joback Method
cpg	181.85	J/mol×K	400.71	Joback Method
cpg	234.50	J/mol×K	554.59	Joback Method
dvisc	0.0003867	Pa×s	369.93	Joback Method
dvisc	0.0004501	Pa×s	339.42	Joback Method
dvisc	0.0005397	Pa×s	308.92	Joback Method
dvisc	0.0006735	Pa×s	278.41	Joback Method
dvisc	0.0008875	Pa×s	247.90	Joback Method
dvisc	0.0012637	Pa×s	217.40	Joback Method
dvisc	0.0020193	Pa×s	186.89	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=C23850784&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
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
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