

Oxirane, (1-methylethyl)-

Other names:	Butane, 1,2-epoxy-3-methyl- Isopropylethylene oxide Isopropyloxirane 2-Isopropyloxirane 3-Methylbutene-1,2-oxide 1-Methylethyl-oxirane 1,2-epoxy-3-methylbutane
Inchi:	InChI=1S/C5H10O/c1-4(2)5-3-6-5/h4-5H,3H2,1-2H3
InchiKey:	REYZXWIIUPKFTI-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC(C)C1CO1
Mol. weight [g/mol]:	86.13
CAS:	1438-14-8

Physical Properties

Property code	Value	Unit	Source
gf	-36.59	kJ/mol	Joback Method
hf	-211.01	kJ/mol	Joback Method
hfus	11.30	kJ/mol	Joback Method
hvap	30.76	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	1.041		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	613.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	613.30		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	627.00		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	613.80		NIST Webbook
rinpol	613.80		NIST Webbook
tb	354.15 ± 3.00	K	NIST Webbook
tc	532.24	K	Joback Method
tf	175.62	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	133.96	J/molxK	347.05	Joback Method
cpg	144.93	J/molxK	377.92	Joback Method
cpg	155.32	J/molxK	408.78	Joback Method
cpg	165.17	J/molxK	439.65	Joback Method
cpg	174.49	J/molxK	470.51	Joback Method
cpg	183.32	J/molxK	501.38	Joback Method
cpg	191.67	J/molxK	532.24	Joback Method
dvisc	0.0015358	Paxs	175.62	Joback Method
dvisc	0.0010067	Paxs	204.19	Joback Method
dvisc	0.0007320	Paxs	232.76	Joback Method
dvisc	0.0005707	Paxs	261.34	Joback Method
dvisc	0.0004673	Paxs	289.91	Joback Method
dvisc	0.0003966	Paxs	318.48	Joback Method
dvisc	0.0003458	Paxs	347.05	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=C1438148&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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