

Oxirane, 2,3-dimethyl-, trans-

Other names:	Butane, 2,3-epoxy-, trans- trans-2-Butene Oxide trans-2-Butylene Oxide trans-2,3-Dimethyloxirane trans-2,3-Epoxybutane 2,3-Butylene oxide (trans) 2,3-Dimethyloxirane, trans 2,3-Dimethyl-oxirane (E)
Inchi:	InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	PQXKWPLDPFFDJP-IMJSIDKUSA-N
Formula:	C4H8O
SMILES:	CC1OC1C
Mol. weight [g/mol]:	72.11
CAS:	21490-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-50.28	kJ/mol	Joback Method
hf	-205.43	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	28.61	kJ/mol	Joback Method
ie	9.98	eV	NIST Webbook
log10ws	-0.70		Crippen Method
logp	0.794		Crippen Method
mcvol	62.230	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	517.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	520.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	543.50		NIST Webbook
rinpol	543.60		NIST Webbook
rinpol	543.70		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	544.00		NIST Webbook

tb	327.50 ± 0.50	K	NIST Webbook
tb	330.15 ± 3.00	K	NIST Webbook
tb	327.70	K	NIST Webbook
tc	499.65	K	Joback Method
tf	190.55 ± 0.50	K	NIST Webbook
tf	188.15 ± 6.00	K	NIST Webbook
vc	0.236	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.87	J/mol×K	319.94	Joback Method
cpg	111.08	J/mol×K	349.89	Joback Method
cpg	119.86	J/mol×K	379.84	Joback Method
cpg	128.23	J/mol×K	409.80	Joback Method
cpg	136.19	J/mol×K	439.75	Joback Method
cpg	143.77	J/mol×K	469.70	Joback Method
cpg	150.98	J/mol×K	499.65	Joback Method
dvisc	0.0003513	Pa×s	175.11	Joback Method
dvisc	0.0003166	Pa×s	199.25	Joback Method
dvisc	0.0002918	Pa×s	223.39	Joback Method
dvisc	0.0002732	Pa×s	247.53	Joback Method
dvisc	0.0002589	Pa×s	271.66	Joback Method
dvisc	0.0002474	Pa×s	295.80	Joback Method
dvisc	0.0002381	Pa×s	319.94	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=C21490631&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
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

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