Oxirane, trimethyl-

Other names:	Butane, 2,3-epoxy-2-methyl-
	«beta»-Isoamylene oxide
	Trimethylethylene oxide
	Trimethyloxacyclopropane
	Trimethyloxirane
	2-Methyl-2-butene oxide
	2-Methyl-2,3-epoxybutane
	2,3-Epoxy-2-methylbutane
	oxirane, 2,2,3-trimethyl-
	2,2,3-Trimethyloxirane
	«alpha»-Trimethylethylene oxide
Inchi:	InChI=1S/C5H10O/c1-4-5(2,3)6-4/h4H,1-3H3
InchiKey:	QPBYBLZYMNWGMO-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC1OC1(C)C
Mol. weight [g/mol]:	86.13
CAS:	5076-19-7

Physical Properties

Property code	Value	Unit	Source
chl	-3133.00	kJ/mol	NIST Webbook
gf	-47.35	kJ/mol	Joback Method
hf	-210.83	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	29.69	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	1.184		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
rinpol	668.00		NIST Webbook
rinpol	668.20		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	649.00		NIST Webbook
rinpol	668.20		NIST Webbook
rinpol	668.10		NIST Webbook
rinpol	668.00		NIST Webbook
rinpol	668.00		NIST Webbook

rinpol	668.00		NIST Webbook
tb	348.65 ± 2.00	K	NIST Webbook
tc	531.54	K	Joback Method
tf	210.28	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.28	J/mol×K	343.06	Joback Method
cpg	146.27	J/mol×K	374.47	Joback Method
cpg	157.32	J/mol×K	405.89	Joback Method
cpg	167.52	J/mol×K	437.30	Joback Method
cpg	176.93	J/mol×K	468.71	Joback Method
cpg	185.65	J/mol×K	500.12	Joback Method
cpg	193.73	J/mol×K	531.54	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=C5076197&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
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