

Oxirane, 2-methyl-2-propyl-

Other names:	Pentane, 1,2-epoxy-2-methyl- 2-Methyl-1-pentene epoxide 2-Methyl-1-pentene oxide 2-Methyl-1,2-epoxypentane 2-Methyl-2-propyl-oxirane
Inchi:	InChI=1S/C6H12O/c1-3-4-6(2)5-7-6/h3-5H2,1-2H3
InchiKey:	FFXMEOKFDOVSGT-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CCCC1(C)CO1
Mol. weight [g/mol]:	100.16
CAS:	3657-41-8

Physical Properties

Property code	Value	Unit	Source
gf	-31.22	kJ/mol	Joback Method
hf	-211.13	kJ/mol	Joback Method
hfus	11.11	kJ/mol	Joback Method
hvap	32.22	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.575		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	736.40		NIST Webbook
rinpol	736.40		NIST Webbook
rinpol	737.80		NIST Webbook
rinpol	737.40		NIST Webbook
rinpol	741.00		NIST Webbook
rinpol	737.80		NIST Webbook
tb	370.61	K	Joback Method
tc	559.20	K	Joback Method
tf	225.79	K	Joback Method
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.98	J/mol×K	370.61	Joback Method
cpg	182.87	J/mol×K	402.04	Joback Method
cpg	194.77	J/mol×K	433.47	Joback Method
cpg	205.76	J/mol×K	464.91	Joback Method
cpg	215.93	J/mol×K	496.34	Joback Method
cpg	225.37	J/mol×K	527.77	Joback Method
cpg	234.15	J/mol×K	559.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3657418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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