

Oxirane, 2-methyl-3-propyl-, trans-

Other names:	Hexane, 2,3-epoxy-, trans- trans-2,3-Epoxyhexane 2,3-epoxyhexane, trans 2-Methyl-3-propyloxirane, (E)- Oxirane, 2-methyl-3-propyl-, (2R,3R)-rel- trans-2-Methyl-3-propyloxirane
Inchi:	InChI=1S/C6H12O/c1-3-4-6-5(2)7-6/h5-6H,3-4H2,1-2H3/t5-,6-/m1/s1
InchiKey:	LIESJAYIOKBLIL-PHDIDXHHSA-N
Formula:	C6H12O
SMILES:	CCCC1OC1C
Mol. weight [g/mol]:	100.16
CAS:	6124-91-0

Physical Properties

Property code	Value	Unit	Source
gf	-33.44	kJ/mol	Joback Method
hf	-246.71	kJ/mol	Joback Method
hfus	18.48	kJ/mol	Joback Method
hvap	33.06	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	1.574		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	739.60		NIST Webbook
rinpol	739.80		NIST Webbook
rinpol	739.60		NIST Webbook
rinpol	739.80		NIST Webbook
tb	365.70	K	Joback Method
tc	545.29	K	Joback Method
tf	197.65	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.05	J/mol×K	365.70	Joback Method
cpg	225.08	J/mol×K	515.36	Joback Method
cpg	215.10	J/mol×K	485.43	Joback Method
cpg	204.63	J/mol×K	455.49	Joback Method
cpg	193.64	J/mol×K	425.56	Joback Method
cpg	182.12	J/mol×K	395.63	Joback Method
cpg	234.59	J/mol×K	545.29	Joback Method
dvisc	0.0003506	Pa×s	365.70	Joback Method
dvisc	0.0003786	Pa×s	337.69	Joback Method
dvisc	0.0004145	Pa×s	309.68	Joback Method
dvisc	0.0004621	Pa×s	281.68	Joback Method
dvisc	0.0005278	Pa×s	253.67	Joback Method
dvisc	0.0006229	Pa×s	225.66	Joback Method
dvisc	0.0007706	Pa×s	197.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6124910&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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