

Oxirane, 2-methyl-3-propyl-, cis-

Other names:	Hexane, 2,3-epoxy-, cis- 2,3-Epoxyhexane, cis 2-Methyl-3-propyl-oxirane, (Z)-
Inchi:	InChI=1S/C6H12O/c1-3-4-6-5(2)7-6/h5-6H,3-4H2,1-2H3/t5-,6+/m0/s1
InchiKey:	LIESJAYIOKBLIL-NTSWFWBYSAN
Formula:	C6H12O
SMILES:	CCCC1OC1C
Mol. weight [g/mol]:	100.16
CAS:	6124-90-9

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	766.90		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	762.20		NIST Webbook
rinpol	766.40		NIST Webbook
rinpol	762.20		NIST Webbook
rinpol	766.90		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	Paxs	365.70	Joback Method
dvisc	0.0003786	Paxs	337.69	Joback Method
dvisc	0.0004145	Paxs	309.68	Joback Method
dvisc	0.0004621	Paxs	281.68	Joback Method
dvisc	0.0005278	Paxs	253.67	Joback Method
dvisc	0.0006229	Paxs	225.66	Joback Method
dvisc	0.0007706	Paxs	197.65	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=C6124909&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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