

Oxirane, 2-methyl-3-(1-methylethyl)-

Other names:	Pentane, 2,3-epoxy-4-methyl- trans-4-methyl-2,3-epoxypentane
Inchi:	InChI=1S/C6H12O/c1-4(2)6-5(3)7-6/h4-6H,1-3H3
InchiKey:	AYTCGOOJNRZGBU-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	CC(C)C1OC1C
Mol. weight [g/mol]:	100.16
CAS:	1192-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-35.88	kJ/mol	Joback Method
hf	-251.99	kJ/mol	Joback Method
hfus	14.96	kJ/mol	Joback Method
hvap	32.68	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	1.430		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	696.20		NIST Webbook
rinpol	695.90		NIST Webbook
rinpol	695.90		NIST Webbook
rinpol	696.60		NIST Webbook
rinpol	696.30		NIST Webbook
tb	365.26	K	Joback Method
tc	549.25	K	Joback Method
tf	182.65	K	Joback Method
vc	0.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.90	J/molxK	365.26	Joback Method
cpg	226.59	J/molxK	518.58	Joback Method

cpg	216.34	J/mol×K	487.92	Joback Method
cpg	205.56	J/mol×K	457.25	Joback Method
cpg	194.25	J/mol×K	426.59	Joback Method
cpg	182.36	J/mol×K	395.92	Joback Method
cpg	236.34	J/mol×K	549.25	Joback Method
dvisc	0.0003404	Paxs	365.26	Joback Method
dvisc	0.0003739	Paxs	334.82	Joback Method
dvisc	0.0004184	Paxs	304.39	Joback Method
dvisc	0.0004800	Paxs	273.95	Joback Method
dvisc	0.0005700	Paxs	243.52	Joback Method
dvisc	0.0007109	Paxs	213.09	Joback Method
dvisc	0.0009543	Paxs	182.65	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=C1192310&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
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

Latest version available from:

<https://www.chemeo.com/cid/73-021-7/Oxirane-2-methyl-3-1-methylethyl.pdf>

Generated by Cheméo on 2024-04-26 17:39:13.064960026 +0000 UTC m=+16442401.985537341.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.