Oxirane, pentyl-

Other names:	1-Heptene oxide
	Heptane, 1,2-epoxy-
	Heptene 1,2-oxide
	Pentyloxirane
	1,2-Epoxyheptane
Inchi:	InChI=1S/C7H14O/c1-2-3-4-5-7-6-8-7/h7H,2-6H2,1H3
InchiKey:	NMOFYYYCFRVWBK-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CCCCCC1CO1
Mol. weight [g/mol]:	114.19
CAS:	5063-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-17.31	kJ/mol	Joback Method
hf	-247.01	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	35.60	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.965		Crippen Method
mcvol	104.500	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	905.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1153.00		NIST Webbook
tb	393.25	K	Joback Method
tc	572.73	K	Joback Method
tf	213.16	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.15	J/mol×K	572.73	Joback Method

cpg	207.56	J/mol×K	393.25	Joback Method
cpg	220.67	J/mol×K	423.16	Joback Method
cpg	233.14	J/mol×K	453.08	Joback Method
cpg	245.00	J/mol×K	482.99	Joback Method
cpg	256.27	J/mol×K	512.90	Joback Method
cpg	266.98	J/mol×K	542.81	Joback Method
dvisc	0.0004314	Pa×s	393.25	Joback Method
dvisc	0.0018616	Pa×s	213.16	Joback Method
dvisc	0.0012553	Pa×s	243.18	Joback Method
dvisc	0.0009230	Pa×s	273.19	Joback Method
dvisc	0.0007213	Pa×s	303.20	Joback Method
dvisc	0.0005892	Pa×s	333.22	Joback Method
dvisc	0.0004977	Pa×s	363.24	Joback Method
hvapt	45.50	kJ/mol	359.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5063650&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
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
hvapt: Enthalpy of vaporization at a given temperature
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
ripol: Polar retention indices

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

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