Oxirane, 2,3-diethyl-

Other names: Hexane, 3,4-epoxy-
3,4-Epoxyhexane
2,3-Diethyloxirane
Inchi: InChI=1S/C6H12O/c1-3-5-6(4-2)7-5/h5-6H,3-4H2,1-2H3
InchiKey: PCGTXZMDZGOMJG-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CCC1OC1CC
Mol. weight [g/mol]: 100.16
CAS: 4468-66-0

Physical Properties

Property code	Value	Unit	Source
chl	-3818.00	kJ/mol	NIST Webbook
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	749.00		NIST Webbook
rinpol	749.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	744.00		NIST Webbook
tb	379.00 ± 2.50	K	NIST Webbook
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=C4468660&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

chl: Standard liquid enthalpy of combustion
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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