

# Oxirane, phenyl-

<b>Other names:</b>	(.+/-)-Styrene oxide (1,2-Epoxyethyl)benzene (Epoxyethyl)benzene 1,2-Epoxy-1-phenylethane 1-Phenyl-1,2-epoxyethane 1-Phenyloxirane 2-Phenyloxirane Benzene, (epoxyethyl)- Benzene, epoxymethyl- Epoxyethylene oxide Epoxyethylene oxide Ethane, 1,2-epoxy-1-phenyl- Fenyloxiran NCI-C54977 NSC 637 Oxirane, 2-phenyl- Phenethylene oxide Phenylethylene oxide Phenyloxirane Styrene 7,8-oxide Styrene epoxide Styrene oxide Styryl oxide «alpha», «beta»-Epoxyethylene oxide Â«alphaÂ», Â«betaÂ»-Epoxyethylene oxide
<b>Inchi:</b>	InChI=1S/C8H8O/c1-2-4-7(5-3-1)8-6-9-8/h1-5,8H,6H2
<b>InchiKey:</b>	AWMVMTVKBNGEAK-UHFFFAOYSA-N
<b>Formula:</b>	C8H8O
<b>SMILES:</b>	c1ccc(C2CO2)cc1
<b>Mol. weight [g/mol]:</b>	120.15
<b>CAS:</b>	96-09-3

## Physical Properties

Property code	Value	Unit	Source
gf	103.52	kJ/mol	Joback Method
hf	-31.12	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method

hvap	40.10		kJ/mol	Joback Method
ie	9.07		eV	NIST Webbook
ie	9.23		eV	NIST Webbook
ie	9.04		eV	NIST Webbook
log10ws	-1.60			Estimated Solubility Method
log10ws	-1.60			Aqueous Solubility Prediction Method
logp	1.758			Crippen Method
mcvol	94.830		ml/mol	McGowan Method
pc	4249.61		kPa	Joback Method
rinpol	1119.00			NIST Webbook
rinpol	1119.00			NIST Webbook
ripol	1628.90			NIST Webbook
ripol	1630.80			NIST Webbook
tb	467.25		K	NIST Webbook
tb	467.30		K	NIST Webbook
tc	670.29		K	Joback Method
tf	236.35		K	NIST Webbook
tf	236.85		K	Aqueous Solubility Prediction Method
vc	0.353		m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.70	J/molxK	442.81	Joback Method
cpg	201.41	J/molxK	480.72	Joback Method
cpg	214.08	J/molxK	518.64	Joback Method
cpg	225.78	J/molxK	556.55	Joback Method
cpg	236.58	J/molxK	594.46	Joback Method
cpg	246.54	J/molxK	632.38	Joback Method
cpg	255.73	J/molxK	670.29	Joback Method
dvisc	0.0018556	Paxs	250.85	Joback Method
dvisc	0.0012889	Paxs	282.84	Joback Method
dvisc	0.0009641	Paxs	314.84	Joback Method
dvisc	0.0007608	Paxs	346.83	Joback Method
dvisc	0.0006249	Paxs	378.82	Joback Method
dvisc	0.0005293	Paxs	410.82	Joback Method
dvisc	0.0004591	Paxs	442.81	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C96093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C96093&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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