Oxirane, phenyl-

Other names:	(.+/-.)-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-
	Epoxystyrene
	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»-Epoxystyrene
	Â«alphaÂ»,Â«betaÂ»-Epoxystyrene
Inchi:	InChI=1S/C8H8O/c1-2-4-7(5-3-1)8-6-9-8/h1-5,8H,6H2
InchiKey:	AWMVMTVKBNGEAK-UHFFFAOYSA-N
Formula:	C8H8O
SMILES:	c1ccc(C2CO2)cc1
Mol. weight [g/mol]:	120.15
CAS:	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	9.04	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
log10ws	-1.60		Aqueous Solubility Prediction Method
log10ws	-1.60		Estimated Solubility 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	236.85	K	Aqueous Solubility Prediction Method
tf	236.35	K	NIST Webbook
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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
ie:	Ionization energy
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