Oxirane, 2-methyl-2-phenyl-

Other names:	Cumene, «alpha»,«beta»-epoxy- «alpha»-Methylstyrene oxide «alpha»-Methylstyrene epoxide Benzene, (1,2-epoxy-1-methylethyl)- Propane, 1,2-epoxy-2-phenyl- Propylene oxide, 2-phenyl- 1-Methyl-1-phenyloxirane 2-Phenyl-1,2-epoxypropane 2-Phenylpropene oxide Cumol, «alpha»,«beta»-epoxy- 2-Methyl-2-phenyloxirane «alpha»-methylepoxystyrene 2-Phenyl-2-methyloxirane NSC 36616 NSC 51065
Inchi:	InChI=1S/C9H10O/c1-9(7-10-9)8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	MRXPNWXSFCODDY-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC1(c2ccccc2)CO1
Mol. weight [g/mol]:	134.18
CAS:	2085-88-3

Physical Properties

Property code	Value	Unit	Source
gf	106.45	kJ/mol	Joback Method
hf	-36.52	kJ/mol	Joback Method
hfus	12.92	kJ/mol	Joback Method
hvap	41.18	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.932		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
ripol	1666.30		NIST Webbook
ripol	1665.50		NIST Webbook
tb	465.93	K	Joback Method
tc	700.22	K	Joback Method
tf	286.02	K	Joback Method

vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.48	J/mol×K	465.93	Joback Method
cpg	244.34	J/mol×K	504.98	Joback Method
cpg	257.78	J/mol×K	544.03	Joback Method
cpg	270.00	J/mol×K	583.07	Joback Method
cpg	281.17	J/mol×K	622.12	Joback Method
cpg	291.47	J/mol×K	661.17	Joback Method
cpg	301.09	J/mol×K	700.22	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2085883&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

cpg: Ideal gas heat capacity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume