

Benzene, 1-chloro-4-(epoxyethyl)-

Other names:	(p-Chlorophenyl)oxirane p-Chlorostyrene oxide 4-Chlorostyrene oxide Oxirane, (4-chlorophenyl)- 4-Chloroepoxystyrene
Inchi:	InChI=1S/C8H7ClO/c9-7-3-1-6(2-4-7)8-5-10-8/h1-4,8H,5H2
InchiKey:	IBWLXNDOMYKTAD-UHFFFAOYSA-N
Formula:	C8H7ClO
SMILES:	Clc1ccc(C2CO2)cc1
Mol. weight [g/mol]:	154.59
CAS:	2788-86-5

Physical Properties

Property code	Value	Unit	Source
gf	81.96	kJ/mol	Joback Method
hf	-58.33	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.411		Crippen Method
mcvol	107.070	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
ripol	1767.30		NIST Webbook
ripol	1767.30		NIST Webbook
ripol	1773.20		NIST Webbook
tb	485.22	K	Joback Method
tc	720.48	K	Joback Method
tf	293.29	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.75	J/mol×K	485.22	Joback Method

cpg	226.02	J/mol×K	524.43	Joback Method
cpg	237.33	J/mol×K	563.64	Joback Method
cpg	247.74	J/mol×K	602.85	Joback Method
cpg	257.33	J/mol×K	642.06	Joback Method
cpg	266.16	J/mol×K	681.27	Joback Method
cpg	274.29	J/mol×K	720.48	Joback Method
dvisc	0.0018468	Pa×s	293.29	Joback Method
dvisc	0.0013529	Pa×s	325.28	Joback Method
dvisc	0.0010478	Pa×s	357.27	Joback Method
dvisc	0.0008464	Pa×s	389.25	Joback Method
dvisc	0.0007062	Pa×s	421.24	Joback Method
dvisc	0.0006045	Pa×s	453.23	Joback Method
dvisc	0.0005281	Pa×s	485.22	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2788865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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