

3-methylepoxystyrene

Inchi:	InChI=1S/C9H10O/c1-7-3-2-4-8(5-7)9-6-10-9/h2-5,9H,6H2,1H3
InchiKey:	HLGUPCNLTKMZDU-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	Cc1ccccc(C2CO2)c1
Mol. weight [g/mol]:	134.18

Physical Properties

Property code	Value	Unit	Source
gf	102.31	kJ/mol	Joback Method
hf	-63.23	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	42.99	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.066		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
ripol	1757.40		NIST Webbook
ripol	1751.40		NIST Webbook
ripol	1757.40		NIST Webbook
tb	470.67	K	Joback Method
tc	696.07	K	Joback Method
tf	274.64	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.43	J/mol×K	470.67	Joback Method
cpg	243.71	J/mol×K	508.24	Joback Method
cpg	256.99	J/mol×K	545.80	Joback Method
cpg	269.35	J/mol×K	583.37	Joback Method
cpg	280.83	J/mol×K	620.94	Joback Method
cpg	291.50	J/mol×K	658.50	Joback Method
cpg	301.42	J/mol×K	696.07	Joback Method

dvisc	0.0016500	Pa×s	274.64	Joback Method
dvisc	0.0011869	Pa×s	307.31	Joback Method
dvisc	0.0009095	Pa×s	339.98	Joback Method
dvisc	0.0007303	Pa×s	372.65	Joback Method
dvisc	0.0006075	Pa×s	405.33	Joback Method
dvisc	0.0005194	Pa×s	438.00	Joback Method
dvisc	0.0004539	Pa×s	470.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R321645&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
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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