3,4-Methylenedioxystyrene

Inchi: InChI=1S/C9H8O2/c1-2-7-3-4-8-9(5-7)11-6-10-8/h2-5H,1,6H2
InchiKey: VWAVZAMMNJMAEM-UHFFFAOYSA-N
Formula: C9H8O2
SMILES: C=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 148.16

Physical Properties

Property code	Value	Unit	Source
gf	102.11	kJ/mol	Joback Method
hf	-60.93	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	47.80	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.058		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
pc	3935.71	kPa	Joback Method
rinpol	1232.00		NIST Webbook
rinpol	1232.00		NIST Webbook
ripol	1852.00		NIST Webbook
tb	503.95	K	Joback Method
tc	734.26	K	Joback Method
tf	316.21	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.79	J/mol×K	503.95	Joback Method
cpg	250.80	J/mol×K	542.33	Joback Method
cpg	261.90	J/mol×K	580.72	Joback Method
cpg	272.15	J/mol×K	619.10	Joback Method
cpg	281.63	J/mol×K	657.49	Joback Method
cpg	290.39	J/mol×K	695.87	Joback Method
cpg	298.52	J/mol×K	734.26	Joback Method

dvisc	0.0019604	Pa×s	316.21	Joback Method
dvisc	0.0013893	Pa×s	347.50	Joback Method
dvisc	0.0010422	Pa×s	378.79	Joback Method
dvisc	0.0008169	Pa×s	410.08	Joback Method
dvisc	0.0006628	Pa×s	441.37	Joback Method
dvisc	0.0005529	Pa×s	472.66	Joback Method
dvisc	0.0004717	Pa×s	503.95	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=R545658&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
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

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