Styrene, «alpha»-(chloromethyl)

Inchi: InChI=1S/C9H7Cl3/c1-7(9(10,11)12)8-5-3-2-4-6-8/h2-6H,1H2
InchiKey: JFRUTHVQVYNYAW-UHFFFAOYSA-N
Formula: C9H7Cl3
SMILES: C=C(c1ccccc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 221.51

Physical Properties

Property code	Value	Unit	Source
gf	183.65	kJ/mol	Joback Method
hf	67.11	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	49.17	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.070		Crippen Method
mcvol	146.330	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1181.00		NIST Webbook
tb	537.62	K	Joback Method
tc	787.32	K	Joback Method
tf	294.07	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.34	J/mol×K	537.62	Joback Method
cpg	290.27	J/mol×K	579.24	Joback Method
cpg	301.03	J/mol×K	620.85	Joback Method
cpg	310.72	J/mol×K	662.47	Joback Method
cpg	319.44	J/mol×K	704.09	Joback Method
cpg	327.29	J/mol×K	745.70	Joback Method
cpg	334.39	J/mol×K	787.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515494&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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