

Benzene, (3-chloro-1-propenyl)-

Other names:	Benzene, (3-chloropropenyl)- Cinnamyl chloride Propene, 3-chloro-1-phenyl- 1-Propene, 3-chloro-1-phenyl- 3-Chloro-1-phenylpropene 3-Phenyl-2-propenyl chloride (3-Chloropropenyl)benzene 1-Phenyl-3-chloro-1-propene 3-Chloro-1-phenyl-1-propene (3-Chloroprop-1-enyl)benzene Benzene, (3-chloro-1-propen-1-yl)- NSC 5599
Inchi:	InChI=1S/C9H9Cl/c10-8-4-7-9-5-2-1-3-6-9/h1-7H,8H2/b7-4+
InchiKey:	IWTYTFSSTWXZFU-QPJJBHSA-N
Formula:	C9H9Cl
SMILES:	C1CC=Cc1ccccc1
Mol. weight [g/mol]:	152.62
CAS:	2687-12-9

Physical Properties

Property code	Value	Unit	Source
gf	205.60	kJ/mol	Joback Method
hf	108.92	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	42.25	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.939		Crippen Method
mcpvol	121.850	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	1262.00		NIST Webbook
tb	473.59	K	Joback Method
tc	698.08	K	Joback Method
tf	242.45	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.60	J/mol×K	473.59	Joback Method
cpg	281.33	J/mol×K	660.66	Joback Method
cpg	271.80	J/mol×K	623.25	Joback Method
cpg	261.52	J/mol×K	585.83	Joback Method
cpg	250.43	J/mol×K	548.42	Joback Method
cpg	238.47	J/mol×K	511.00	Joback Method
cpg	290.16	J/mol×K	698.08	Joback Method
dvisc	0.0002156	Pa×s	473.59	Joback Method
dvisc	0.0002770	Pa×s	435.07	Joback Method
dvisc	0.0003735	Pa×s	396.54	Joback Method
dvisc	0.0005371	Pa×s	358.02	Joback Method
dvisc	0.0008430	Pa×s	319.50	Joback Method
dvisc	0.0014975	Pa×s	280.97	Joback Method
dvisc	0.0031929	Pa×s	242.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	1.60	NIST Webbook

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=C2687129&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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