Benzene, (3-chloroallyl)-

Other names: Benzene, (3-chloro-2-propenyl)-
Inchi: InChI=1S/C9H9Cl/c10-8-4-7-9-5-2-1-3-6-9/h1-6,8H,7H2/b8-4+
InchiKey: JJTUJRVKTPSEFZ-XBXARRHUSA-N
Formula: C9H9Cl
SMILES: ClC=CCc1ccccc1
Mol. weight [g/mol]: 152.62
CAS: 6268-37-7

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	-3.19		Crippen Method
logp	2.982		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
tb	486.20	K	NIST Webbook
tb	481.65 ± 2.00	K	NIST Webbook
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	238.47	J/mol×K	511.00	Joback Method
cpg	250.43	J/mol×K	548.42	Joback Method
cpg	261.52	J/mol×K	585.83	Joback Method
cpg	271.80	J/mol×K	623.25	Joback Method
cpg	281.33	J/mol×K	660.66	Joback Method
cpg	290.16	J/mol×K	698.08	Joback Method

dvisc	0.0031929	Pa×s	242.45	Joback Method
dvisc	0.0014975	Pa×s	280.97	Joback Method
dvisc	0.0008430	Pa×s	319.50	Joback Method
dvisc	0.0005371	Pa×s	358.02	Joback Method
dvisc	0.0003735	Pa×s	396.54	Joback Method
dvisc	0.0002770	Pa×s	435.07	Joback Method
dvisc	0.0002156	Pa×s	473.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.20	K	2.40	NIST Webbook

Sources

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=C6268377&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume