3-Bromo-1-phenyl-1-propene

Other names: 3-Bromo-1-phenyl propene-1
Cinnamyl bromide
[3-Bromo-1-propenyl]benzene
Inchi: InChI=1S/C9H9Br/c10-8-4-7-9-5-2-1-3-6-9/h1-7H,8H2/b7-4+
InchiKey: RUROFEVDCUGKHD-QPJJXVBHSA-N
Formula: C9H9Br
SMILES: BrCC=Cc1ccccc1
Mol. weight [g/mol]: 197.07
CAS: 4392-24-9

Physical Properties

Property code	Value	Unit	Source
gf	231.85	kJ/mol	Joback Method
hf	150.99	kJ/mol	Joback Method
hfus	18.59	kJ/mol	Joback Method
hvap	44.30	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	3.095		Crippen Method
mcvol	127.110	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	502.32	K	Joback Method
tc	738.17	K	Joback Method
tf	272.33	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.96	J/mol×K	502.32	Joback Method
cpg	249.66	J/mol×K	541.63	Joback Method
cpg	261.36	J/mol×K	580.94	Joback Method
cpg	272.15	J/mol×K	620.24	Joback Method
cpg	282.08	J/mol×K	659.55	Joback Method
cpg	291.24	J/mol×K	698.86	Joback Method

cpg	299.70	J/mol×K	738.17	Joback Method
dvisc	0.0027272	Pa×s	272.33	Joback Method
dvisc	0.0014124	Pa×s	310.66	Joback Method
dvisc	0.0008452	Pa×s	348.99	Joback Method
dvisc	0.0005599	Pa×s	387.33	Joback Method
dvisc	0.0003994	Pa×s	425.66	Joback Method
dvisc	0.0003013	Pa×s	463.99	Joback Method
dvisc	0.0002373	Pa×s	502.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	2.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4392249&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

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