

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	m ³ /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	Paxs	272.33	Joback Method
dvisc	0.0014124	Paxs	310.66	Joback Method
dvisc	0.0008452	Paxs	348.99	Joback Method
dvisc	0.0005599	Paxs	387.33	Joback Method
dvisc	0.0003994	Paxs	425.66	Joback Method
dvisc	0.0003013	Paxs	463.99	Joback Method
dvisc	0.0002373	Paxs	502.32	Joback Method

Pressure Dependent Properties

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

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=C4392249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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