

Benzene, 1-bromo-2-ethenyl-

Other names:	o-Bromostyrene 2-Bromostyrene o-Bromovinylbenzene Styrene, o-bromo-
Inchi:	InChI=1S/C8H7Br/c1-2-7-5-3-4-6-8(7)9/h2-6H,1H2
InchiKey:	SSZOCHFYYWWVSAI-UHFFFAOYSA-N
Formula:	C8H7Br
SMILES:	C=Cc1ccccc1Br
Mol. weight [g/mol]:	183.04
CAS:	2039-88-5

Physical Properties

Property code	Value	Unit	Source
gf	221.42	kJ/mol	Joback Method
hf	168.37	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.092		Crippen Method
mcvol	113.020	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	482.40	K	NIST Webbook
tc	712.22	K	Joback Method
tf	220.40 ± 0.05	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.05	J/mol×K	476.94	Joback Method
cpg	206.94	J/mol×K	516.15	Joback Method
cpg	217.04	J/mol×K	555.37	Joback Method
cpg	226.38	J/mol×K	594.58	Joback Method
cpg	235.03	J/mol×K	633.79	Joback Method

cpg	243.03	J/mol×K	673.00	Joback Method
cpg	250.42	J/mol×K	712.22	Joback Method
dvisc	0.0019793	Pa×s	276.90	Joback Method
dvisc	0.0012112	Pa×s	310.24	Joback Method
dvisc	0.0008153	Pa×s	343.58	Joback Method
dvisc	0.0005886	Pa×s	376.92	Joback Method
dvisc	0.0004480	Pa×s	410.26	Joback Method
dvisc	0.0003553	Pa×s	443.60	Joback Method
dvisc	0.0002911	Pa×s	476.94	Joback Method
hvapt	48.70	kJ/mol	460.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.20	K	2.90	NIST Webbook
tbrp	371.20	K	2.70	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=C2039885&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
hvapt:	Enthalpy of vaporization at a given temperature
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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