

Benzene, 1-bromo-3-iodo-

Other names:	m-Bromiodobenzene 1-Bromo-3-iodobenzene 3-Bromiodobenzene
Inchi:	InChI=1S/C6H4BrI/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	CTPUUDQIXKUAMO-UHFFFAOYSA-N
Formula:	C6H4BrI
SMILES:	Brc1cccc(I)c1
Mol. weight [g/mol]:	282.90
CAS:	591-18-4

Physical Properties

Property code	Value	Unit	Source
gf	174.86	kJ/mol	Joback Method
hf	161.09	kJ/mol	Joback Method
hfus	14.64	kJ/mol	Joback Method
hvap	47.70	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.054		Crippen Method
mcvol	114.960	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	527.64	K	Joback Method
tc	804.32	K	Joback Method
tf	263.85 ± 0.50	K	NIST Webbook
tf	264.00 ± 1.50	K	NIST Webbook
vc	0.413	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.93	J/mol×K	758.21	Joback Method
cpg	198.65	J/mol×K	712.10	Joback Method
cpg	192.82	J/mol×K	665.98	Joback Method
cpg	186.35	J/mol×K	619.87	Joback Method
cpg	179.16	J/mol×K	573.75	Joback Method

cpg	171.17	J/molxK	527.64	Joback Method
cpg	208.72	J/molxK	804.32	Joback Method
cpl	183.10	J/molxK	298.15	NIST Webbook
dvisc	0.0023919	Paxs	314.18	Joback Method
dvisc	0.0003477	Paxs	527.64	Joback Method
dvisc	0.0004269	Paxs	492.06	Joback Method
dvisc	0.0005411	Paxs	456.49	Joback Method
dvisc	0.0007141	Paxs	420.91	Joback Method
dvisc	0.0009918	Paxs	385.33	Joback Method
dvisc	0.0014728	Paxs	349.76	Joback Method
hfust	12.19	kJ/mol	263.85	NIST Webbook
hfust	12.16	kJ/mol	282.50	NIST Webbook
sfust	46.20	J/molxK	263.85	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	525.20	K	101.00	NIST Webbook
tbrp	393.20	K	2.40	NIST Webbook
tbrp	393.00	K	2.40	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=C591184&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
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
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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