

Benzene, 1-bromo-3,5-dichloro-

Other names:	1-Bromo-3,5-dichlorobenzene 3,5-Dichlorobromobenzene
Inchi:	InChI=1S/C6H3BrCl2/c7-4-1-5(8)3-6(9)2-4/h1-3H
InchiKey:	DZHFFMWJXJBBERG-UHFFFAOYSA-N
Formula:	C6H3BrCl2
SMILES:	Clc1cc(Cl)cc(Br)c1
Mol. weight [g/mol]:	225.90
CAS:	19752-55-7

Physical Properties

Property code	Value	Unit	Source
gf	83.25	kJ/mol	Joback Method
hf	41.27	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.756		Crippen Method
mvol	113.620	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	505.00	K	NIST Webbook
tc	765.53	K	Joback Method
tf	356.00 ± 1.00	K	NIST Webbook
vc	0.423	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.54	J/mol×K	514.34	Joback Method
cpg	182.63	J/mol×K	556.21	Joback Method
cpg	189.15	J/mol×K	598.07	Joback Method
cpg	195.13	J/mol×K	639.94	Joback Method
cpg	200.60	J/mol×K	681.80	Joback Method
cpg	205.61	J/mol×K	723.67	Joback Method
cpg	210.20	J/mol×K	765.53	Joback Method

dvisc	0.0015755	Paxs	328.48	Joback Method
dvisc	0.0010816	Paxs	359.46	Joback Method
dvisc	0.0007882	Paxs	390.43	Joback Method
dvisc	0.0006017	Paxs	421.41	Joback Method
dvisc	0.0004767	Paxs	452.39	Joback Method
dvisc	0.0003891	Paxs	483.36	Joback Method
dvisc	0.0003254	Paxs	514.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	505.20	K	101.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19752557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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