

1-Bromo-2,3-dichlorobenzene

Other names:	Benzene, 1-bromo-2,3-dichloro-
Inchi:	InChI=1S/C6H3BrCl2/c7-4-2-1-3-5(8)6(4)9/h1-3H
InchiKey:	HVKCZUVMQPUWSX-UHFFFAOYSA-N
Formula:	C6H3BrCl2
SMILES:	Clc1cccc(Br)c1Cl
Mol. weight [g/mol]:	225.90
CAS:	56961-77-4

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
mcvol	113.620	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
tb	516.00	K	NIST Webbook
tc	765.53	K	Joback Method
tf	333.00	K	NIST Webbook
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.54	J/molxK	514.34	Joback Method
cpg	182.63	J/molxK	556.21	Joback Method
cpg	189.15	J/molxK	598.07	Joback Method
cpg	195.13	J/molxK	639.94	Joback Method
cpg	200.60	J/molxK	681.80	Joback Method
cpg	205.61	J/molxK	723.67	Joback Method
cpg	210.20	J/molxK	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	516.20	K	102.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56961774&Units=SI

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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