1-Bromo-2,4-dichlorobenzene

Other names: Benzene, 1-bromo-2,4-dichloro-
Inchi: InChI=1S/C6H3BrCl2/c7-5-2-1-4(8)3-6(5)9/h1-3H
InchiKey: ISHYFWKKWKXXPL-UHFFFAOYSA-N
Formula: C6H3BrCl2
SMILES: Clc1ccc(Br)c(Cl)c1
Mol. weight [g/mol]: 225.90
CAS: 1193-72-2

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	508.00	K	NIST Webbook
tb	508.20	K	NIST Webbook
tc	765.53	K	Joback Method
tf	298.00	K	NIST Webbook
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

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

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	2.80	NIST Webbook
tbrp	384.00	K	2.80	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=C1193722&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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