

2-bromo-4,6-dichlorophenol

Inchi:	InChI=1S/C6H3BrCl2O/c7-4-1-3(8)2-5(9)6(4)10/h1-2,10H
InchiKey:	FRPHJINKMDMSPH-UHFFFAOYSA-N
Formula:	C6H3BrCl2O
SMILES:	Oc1c(Cl)cc(Cl)cc1Br
Mol. weight [g/mol]:	241.90
CAS:	4524-77-0

Physical Properties

Property code	Value	Unit	Source
gf	-71.37	kJ/mol	Joback Method
hf	-136.04	kJ/mol	Joback Method
hfus	24.02	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.462		Crippen Method
mcvol	119.490	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
tb	594.96	K	Joback Method
tc	857.43	K	Joback Method
tf	341.00	K	NIST Webbook
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.05	J/molxK	857.43	Joback Method
cpg	209.03	J/molxK	594.96	Joback Method
cpg	214.88	J/molxK	638.71	Joback Method
cpg	220.18	J/molxK	682.45	Joback Method
cpg	225.03	J/molxK	726.20	Joback Method
cpg	229.55	J/molxK	769.94	Joback Method
cpg	233.85	J/molxK	813.69	Joback Method
dvisc	0.0000546	Paxs	594.96	Joback Method
dvisc	0.0005619	Paxs	440.20	Joback Method

dvisc	0.0003421	Paxs	465.99	Joback Method
dvisc	0.0002194	Paxs	491.79	Joback Method
dvisc	0.0001471	Paxs	517.58	Joback Method
dvisc	0.0001024	Paxs	543.37	Joback Method
dvisc	0.0000737	Paxs	569.17	Joback Method
hvapt	58.60	kJ/mol	449.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	493.20	K	26.70	NIST Webbook
tbrp	493.00	K	26.70	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=C4524770&Units=SI&Mask=3FFF
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
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

Latest version available from:

<https://www.cheméo.com/cid/111-967-5/2-bromo-4-6-dichlorophenol.pdf>

Generated by Cheméo on 2024-04-29 11:54:13.525979276 +0000 UTC m=+16680902.446556588.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.