2-Bromo-4-chloroanisole

Other names: Benzene, 2-bromo-4-chloro-1-methoxy-
Inchi: InChI=1S/C7H6BrClO/c1-10-7-3-2-5(9)4-6(7)8/h2-4H,1H3
InchiKey: YJEMGEBDXDPBSP-UHFFFAOYSA-N
Formula: C7H6BrClO
SMILES: COc1ccc(Cl)cc1Br
Mol. weight [g/mol]: 221.48
CAS: 60633-25-2

Physical Properties

Property code	Value	Unit	Source
gf	-1.40	kJ/mol	Joback Method
hf	-95.85	kJ/mol	Joback Method
hfus	17.82	kJ/mol	Joback Method
hvap	48.01	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.111		Crippen Method
mcvol	121.340	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	522.21	K	Joback Method
tc	760.14	K	Joback Method
tf	332.06	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.29	J/mol×K	522.21	Joback Method
cpg	224.41	J/mol×K	561.87	Joback Method
cpg	232.98	J/mol×K	601.52	Joback Method
cpg	241.01	J/mol×K	641.18	Joback Method
cpg	248.53	J/mol×K	680.83	Joback Method
cpg	255.53	J/mol×K	720.49	Joback Method
cpg	262.05	J/mol×K	760.14	Joback Method

dvisc	0.0012612	Pa×s	332.06	Joback Method
dvisc	0.0008556	Pa×s	363.75	Joback Method
dvisc	0.0006177	Pa×s	395.44	Joback Method
dvisc	0.0004681	Pa×s	427.13	Joback Method
dvisc	0.0003685	Pa×s	458.83	Joback Method
dvisc	0.0002993	Pa×s	490.52	Joback Method
dvisc	0.0002492	Pa×s	522.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60633252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume