

4-Bromo-2-chloroanisole

Inchi:	InChI=1S/C7H6BrClO/c1-10-7-3-2-5(8)4-6(7)9/h2-4H,1H3
InchiKey:	FPIQNBOUYZLESW-UHFFFAOYSA-N
Formula:	C7H6BrClO
SMILES:	COc1ccc(Br)cc1Cl
Mol. weight [g/mol]:	221.48
CAS:	50638-47-6

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
mvol	121.340	ml/mol	McGowan Method
pc	4036.37	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	522.21	K	Joback Method
tc	760.14	K	Joback Method
tf	332.06	K	Joback Method
vc	0.449	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

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=C50638476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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