

3-Bromo-2,4-dichloroanisole

Inchi:	InChI=1S/C7H5BrCl2O/c1-11-5-3-2-4(9)6(8)7(5)10/h2-3H,1H3
InchiKey:	OXINPOQPENRUHL-UHFFFAOYSA-N
Formula:	C7H5BrCl2O
SMILES:	COc1ccc(Cl)c(Br)c1Cl
Mol. weight [g/mol]:	255.92

Physical Properties

Property code	Value	Unit	Source
gf	-22.96	kJ/mol	Joback Method
hf	-123.06	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.764		Crippen Method
mvol	133.580	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	1444.00		NIST Webbook
rinpol	1444.00		NIST Webbook
tb	564.62	K	Joback Method
tc	808.13	K	Joback Method
tf	374.50	K	Joback Method
vc	0.497	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.46	J/molxK	564.62	Joback Method
cpg	270.24	J/molxK	767.54	Joback Method
cpg	264.05	J/molxK	726.96	Joback Method
cpg	257.38	J/molxK	686.37	Joback Method
cpg	250.24	J/molxK	645.79	Joback Method
cpg	242.60	J/molxK	605.20	Joback Method
cpg	275.96	J/molxK	808.13	Joback Method
dvisc	0.0002358	Paxs	564.62	Joback Method

dvisc	0.0002790	Paxs	532.93	Joback Method
dvisc	0.0003373	Paxs	501.25	Joback Method
dvisc	0.0004183	Paxs	469.56	Joback Method
dvisc	0.0005351	Paxs	437.87	Joback Method
dvisc	0.0007114	Paxs	406.19	Joback Method
dvisc	0.0009926	Paxs	374.50	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=R323592&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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