

2,6-Dibromo-3-chloroanisole

Inchi:	InChI=1S/C7H5Br2ClO/c1-11-7-4(8)2-3-5(10)6(7)9/h2-3H,1H3
InchiKey:	AHBGIHFKTBTQJP-UHFFFAOYSA-N
Formula:	C7H5Br2ClO
SMILES:	COc1c(Br)ccc(Cl)c1Br
Mol. weight [g/mol]:	300.38

Physical Properties

Property code	Value	Unit	Source
gf	3.29	kJ/mol	Joback Method
hf	-80.99	kJ/mol	Joback Method
hfus	22.71	kJ/mol	Joback Method
hvap	55.10	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.874		Crippen Method
mcvol	138.840	ml/mol	McGowan Method
pc	4328.25	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1624.00		NIST Webbook
tb	593.35	K	Joback Method
tc	846.92	K	Joback Method
tf	404.38	K	Joback Method
vc	0.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.49	J/mol×K	593.35	Joback Method
cpg	249.47	J/mol×K	635.61	Joback Method
cpg	256.90	J/mol×K	677.87	Joback Method
cpg	263.80	J/mol×K	720.14	Joback Method
cpg	270.20	J/mol×K	762.40	Joback Method
cpg	276.11	J/mol×K	804.66	Joback Method
cpg	281.56	J/mol×K	846.92	Joback Method

dvisc	0.0008993	Paxs	404.38	Joback Method
dvisc	0.0006623	Paxs	435.88	Joback Method
dvisc	0.0005082	Paxs	467.37	Joback Method
dvisc	0.0004033	Paxs	498.87	Joback Method
dvisc	0.0003289	Paxs	530.36	Joback Method
dvisc	0.0002745	Paxs	561.86	Joback Method
dvisc	0.0002335	Paxs	593.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mvol:	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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