4-Bromo-2,6-dichloroanisole

Inchi: InChI=1S/C7H5BrCl2O/c1-11-7-5(9)2-4(8)3-6(7)10/h2-3H,1H3
InchiKey: OAYSFAKCFYRCRU-UHFFFAOYSA-N
Formula: C7H5BrCl2O
SMILES: COc1c(Cl)cc(Br)cc1Cl
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
mcvol	133.580	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	1427.00		NIST Webbook
rinpol	1427.00		NIST Webbook
tb	564.62	K	Joback Method
tc	808.13	K	Joback Method
tf	374.50	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002790	Pa×s	532.93	Joback Method
dvisc	0.0003373	Pa×s	501.25	Joback Method
dvisc	0.0004183	Pa×s	469.56	Joback Method
dvisc	0.0005351	Pa×s	437.87	Joback Method
dvisc	0.0007114	Pa×s	406.19	Joback Method
dvisc	0.0009926	Pa×s	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=R323636&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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