4-Bromo-2,3,6-trichloroanisole

Inchi: InChI=1S/C7H4BrCl3O/c1-12-7-4(9)2-3(8)5(10)6(7)11/h2H,1H3
InchiKey: VZRSUQWPXPUWCS-UHFFFAOYSA-N
Formula: C7H4BrCl3O
SMILES: COc1c(Cl)cc(Br)c(Cl)c1Cl
Mol. weight [g/mol]: 290.37

Physical Properties

Property code	Value	Unit	Source
gf	-44.52	kJ/mol	Joback Method
hf	-150.27	kJ/mol	Joback Method
hfus	25.43	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.418		Crippen Method
mcvol	145.820	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	607.03	K	Joback Method
tc	855.20	K	Joback Method
tf	416.94	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.78	J/mol×K	607.03	Joback Method
cpg	259.00	J/mol×K	648.39	Joback Method
cpg	265.77	J/mol×K	689.75	Joback Method
cpg	272.08	J/mol×K	731.11	Joback Method
cpg	277.94	J/mol×K	772.48	Joback Method
cpg	283.35	J/mol×K	813.84	Joback Method
cpg	288.31	J/mol×K	855.20	Joback Method
dvisc	0.0007963	Pa×s	416.94	Joback Method

dvisc	0.0005952	Pa×s	448.62	Joback Method
dvisc	0.0004623	Pa×s	480.30	Joback Method
dvisc	0.0003705	Pa×s	511.99	Joback Method
dvisc	0.0003046	Pa×s	543.67	Joback Method
dvisc	0.0002560	Pa×s	575.35	Joback Method
dvisc	0.0002190	Pa×s	607.03	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323621&Units=SI

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