4-Bromo-2,3,5,6-tetrachloroanisole

Inchi: InChI=1S/C7H3BrCl4O/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h1H3
InchiKey: YSVAURKXNCNUNS-UHFFFAOYSA-N
Formula: C7H3BrCl4O
SMILES: COc1c(Cl)c(Cl)c(Br)c(Cl)c1Cl
Mol. weight [g/mol]: 324.81

Physical Properties

Property code	Value	Unit	Source
gf	-66.08	kJ/mol	Joback Method
hf	-177.48	kJ/mol	Joback Method
hfus	29.24	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	5.071		Crippen Method
mcvol	158.060	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	1836.00		NIST Webbook
tb	649.44	K	Joback Method
tc	901.50	K	Joback Method
tf	459.38	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.46	J/mol×K	649.44	Joback Method
cpg	295.05	J/mol×K	859.49	Joback Method
cpg	290.39	J/mol×K	817.48	Joback Method
cpg	285.30	J/mol×K	775.47	Joback Method
cpg	279.78	J/mol×K	733.46	Joback Method
cpg	273.83	J/mol×K	691.45	Joback Method
cpg	299.26	J/mol×K	901.50	Joback Method
dvisc	0.0002006	Pa×s	649.44	Joback Method
dvisc	0.0002319	Pa×s	617.76	Joback Method

dvisc	0.0002724	Pa×s	586.09	Joback Method
dvisc	0.0003259	Pa×s	554.41	Joback Method
dvisc	0.0003984	Pa×s	522.73	Joback Method
dvisc	0.0004999	Pa×s	491.06	Joback Method
dvisc	0.0006472	Pa×s	459.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323616&Units=SI
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

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