2,3,5,6-Tetrabromo-4-methylphenol

Inchi: InChI=1S/C7H4Br4O/c1-2-3(8)5(10)7(12)6(11)4(2)9/h12H,1H3
InchiKey: OMVMKSWFUQZIFD-UHFFFAOYSA-N
Formula: C7H4Br4O
SMILES: Cc1c(Br)c(Br)c(O)c(Br)c1Br
Mol. weight [g/mol]: 423.72

Physical Properties

Property code	Value	Unit	Source
hfus	33.29	kJ/mol	Joback Method
ie	8.20	eV	Cheméo Relay (1.0)
logp	4.751		Crippen Method
mcvol	161.600	ml/mol	McGowan Method
tb	602.32	K	Cheméo Relay (1.0)
tf	483.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.79	J/mol×K	751.42	Joback Method
cpg	284.31	J/mol×K	799.27	Joback Method
cpg	289.74	J/mol×K	847.13	Joback Method
cpg	295.25	J/mol×K	894.98	Joback Method
cpg	301.01	J/mol×K	942.83	Joback Method
cpg	307.21	J/mol×K	990.68	Joback Method
cpg	314.02	J/mol×K	1038.54	Joback Method
dvisc	0.0000827	Pa×s	596.07	Joback Method
dvisc	0.0000606	Pa×s	621.96	Joback Method
dvisc	0.0000455	Pa×s	647.85	Joback Method
dvisc	0.0000350	Pa×s	673.75	Joback Method
dvisc	0.0000274	Pa×s	699.64	Joback Method
dvisc	0.0000218	Pa×s	725.53	Joback Method
dvisc	0.0000177	Pa×s	751.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37721758&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point