2,3,4,6-Tetrabromophenol

Inchi: InChI=1S/C6H2Br4O/c7-2-1-3(8)6(11)5(10)4(2)9/h1,11H
InchiKey: CXPJZISGVIVNEL-UHFFFAOYSA-N
Formula: C6H2Br4O
SMILES: Oc1c(Br)cc(Br)c(Br)c1Br
Mol. weight [g/mol]: 409.69

Physical Properties

Property code	Value	Unit	Source
gf	-14.18	kJ/mol	Joback Method
hf	-37.04	kJ/mol	Joback Method
hfus	31.09	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.442		Crippen Method
mcvol	147.510	ml/mol	McGowan Method
pc	8525.96	kPa	Joback Method
rinpol	265.58		NIST Webbook
tb	723.56	K	Joback Method
tc	1017.96	K	Joback Method
tf	572.28	K	Joback Method
vc	0.477	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.68	J/mol×K	723.56	Joback Method
cpg	256.47	J/mol×K	968.90	Joback Method
cpg	251.56	J/mol×K	919.83	Joback Method
cpg	247.12	J/mol×K	870.76	Joback Method
cpg	242.96	J/mol×K	821.69	Joback Method
cpg	238.88	J/mol×K	772.63	Joback Method
cpg	262.07	J/mol×K	1017.96	Joback Method
dvisc	0.0000225	Pa×s	723.56	Joback Method
dvisc	0.0000280	Pa×s	698.35	Joback Method

dvisc	0.0000354	Pa×s	673.13	Joback Method
dvisc	0.0000457	Pa×s	647.92	Joback Method
dvisc	0.0000602	Pa×s	622.71	Joback Method
dvisc	0.0000812	Pa×s	597.49	Joback Method
dvisc	0.0001123	Pa×s	572.28	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=R504835&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

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