

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

Inchi:	InChI=1S/C6HBr4ClO/c7-1-3(9)6(12)4(10)2(8)5(1)11/h12H
InchiKey:	HHPGOBVKUZQECQ-UHFFFAOYSA-N
Formula:	C6HBr4ClO
SMILES:	Oc1c(Br)c(Br)c(Cl)c(Br)c1Br
Mol. weight [g/mol]:	444.14
CAS:	20188-28-7

Physical Properties

Property code	Value	Unit	Source
gf	-35.74	kJ/mol	Joback Method
hf	-64.25	kJ/mol	Joback Method
hfus	34.90	kJ/mol	Joback Method
hvap	77.01	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.096		Crippen Method
mcvol	159.750	ml/mol	McGowan Method
pc	7762.62	kPa	Joback Method
tb	765.97	K	Joback Method
tc	1061.89	K	Joback Method
tf	614.72	K	Joback Method
vc	0.526	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.36	J/mol×K	765.97	Joback Method
cpg	249.03	J/mol×K	815.29	Joback Method
cpg	252.80	J/mol×K	864.61	Joback Method
cpg	256.85	J/mol×K	913.93	Joback Method
cpg	261.37	J/mol×K	963.25	Joback Method
cpg	266.56	J/mol×K	1012.57	Joback Method
cpg	272.60	J/mol×K	1061.89	Joback Method
dvisc	0.0000712	Paxs	614.72	Joback Method
dvisc	0.0000533	Paxs	639.93	Joback Method

dvisc	0.0000408	Paxs	665.14	Joback Method
dvisc	0.0000318	Paxs	690.35	Joback Method
dvisc	0.0000252	Paxs	715.55	Joback Method
dvisc	0.0000203	Paxs	740.76	Joback Method
dvisc	0.0000166	Paxs	765.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C20188287&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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