1,2,4,6,7,9-hexabromo-dibenzo-dioxin

Inchi: InChI=1S/C12H2Br6O2/c13-3-1-5(15)9-11(7(3)17)20-10-6(16)2-4(14)8(18)12(10)19-9/h1
InchiKey: LFCXBJLENYNRHW-UHFFFAOYSA-N
Formula: C12H2Br6O2
SMILES: Brc1cc(Br)c2c(c1Br)Oc1c(Br)cc(Br)c(Br)c1O2
Mol. weight [g/mol]: 657.57

Physical Properties

Property code	Value	Unit	Source
gf	192.18	kJ/mol	Joback Method
hf	83.57	kJ/mol	Joback Method
hfus	58.64	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	8.160		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
rinpol	3428.00		NIST Webbook
rinpol	3428.00		NIST Webbook
tb	1025.16	K	Joback Method
tc	1336.99	K	Joback Method
tf	815.64	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.63	J/mol×K	1025.16	Joback Method
cpg	500.46	J/mol×K	1285.02	Joback Method
cpg	486.42	J/mol×K	1233.05	Joback Method
cpg	474.20	J/mol×K	1181.08	Joback Method
cpg	463.50	J/mol×K	1129.10	Joback Method
cpg	454.07	J/mol×K	1077.13	Joback Method
cpg	516.60	J/mol×K	1336.99	Joback Method
dvisc	0.0002201	Pa×s	1025.16	Joback Method

dvisc	0.0002421	Pa×s	990.24	Joback Method
dvisc	0.0002683	Pa×s	955.32	Joback Method
dvisc	0.0002996	Pa×s	920.40	Joback Method
dvisc	0.0003374	Pa×s	885.48	Joback Method
dvisc	0.0003838	Pa×s	850.56	Joback Method
dvisc	0.0004414	Pa×s	815.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172344&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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