

Dibenzodioxin, 1,2,3,4,7,8-hexabromo-

Other names:	1,2,3,4,7,8-hexabromo-dibenzo-p-dioxin
Inchi:	InChI=1S/C12H2Br6O2/c13-3-1-5-6(2-4(3)14)20-12-10(18)8(16)7(15)9(17)11(12)19-5/h1
InchiKey:	JGZILVYVJLWSIH-UHFFFAOYSA-N
Formula:	C12H2Br6O2
SMILES:	BrC1cc2c(cc1Br)Oc1c(Br)c(Br)c(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
mcpvol	238.300	ml/mol	McGowan Method
pc	5972.16	kPa	Joback Method
rinpol	3534.00		NIST Webbook
rinpol	3534.00		NIST Webbook
rinpol	3534.00		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/molxK	1025.16	Joback Method
cpg	500.46	J/molxK	1285.02	Joback Method
cpg	486.42	J/molxK	1233.05	Joback Method
cpg	474.20	J/molxK	1181.08	Joback Method
cpg	463.50	J/molxK	1129.10	Joback Method
cpg	454.07	J/molxK	1077.13	Joback Method

cpg	516.60	J/molxK	1336.99	Joback Method
dvisc	0.0002201	Paxs	1025.16	Joback Method
dvisc	0.0002421	Paxs	990.24	Joback Method
dvisc	0.0002683	Paxs	955.32	Joback Method
dvisc	0.0002996	Paxs	920.40	Joback Method
dvisc	0.0003374	Paxs	885.48	Joback Method
dvisc	0.0003838	Paxs	850.56	Joback Method
dvisc	0.0004414	Paxs	815.64	Joback Method

Sources

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=R170462&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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