

3,9-dibromo-1,2,6,7-tetrachloro-dibenzo-p-dioxin

Other names:	Dibenzodioxin, 3,9-dibromo-, 1,2,6,7-tetrachloro-
Inchi:	InChI=1S/C12H2Br2Cl4O2/c13-3-2-6-11(9(18)7(3)16)20-10-4(14)1-5(15)8(17)12(10)19-6
InchiKey:	SNUAUHKBKRXDJBT-UHFFFAOYSA-N
Formula:	C12H2Br2Cl4O2
SMILES:	Clc1cc(Br)c2c(c1Cl)Oc1cc(Br)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]:	479.76

Physical Properties

Property code	Value	Unit	Source
gf	87.18	kJ/mol	Joback Method
hf	-84.71	kJ/mol	Joback Method
hfus	54.29	kJ/mol	Joback Method
hvap	91.63	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.723		Crippen Method
mcvol	217.260	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	910.24	K	Joback Method
tc	1195.12	K	Joback Method
tf	696.12	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.85	J/molxK	910.24	Joback Method
cpg	433.11	J/molxK	957.72	Joback Method
cpg	439.29	J/molxK	1005.20	Joback Method
cpg	445.52	J/molxK	1052.68	Joback Method
cpg	451.96	J/molxK	1100.16	Joback Method
cpg	458.74	J/molxK	1147.64	Joback Method
cpg	466.02	J/molxK	1195.12	Joback Method

dvisc	0.0007377	Paxs	696.12	Joback Method
dvisc	0.0006269	Paxs	731.81	Joback Method
dvisc	0.0005408	Paxs	767.49	Joback Method
dvisc	0.0004727	Paxs	803.18	Joback Method
dvisc	0.0004180	Paxs	838.87	Joback Method
dvisc	0.0003733	Paxs	874.55	Joback Method
dvisc	0.0003364	Paxs	910.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172146&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

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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