

Dibenzodioxin, 1,2,3-tribromo-, 7,8-dichloro-

Other names:	1,2,3-tribromo-7,8-dichlorodibenzo-p-dioxin
Inchi:	InChI=1S/C12H3Br3Cl2O2/c13-4-1-9-12(11(15)10(4)14)19-8-3-6(17)5(16)2-7(8)18-9/h1-
InchiKey:	HJEFXNGPSIEWDU-UHFFFAOYSA-N
Formula:	C12H3Br3Cl2O2
SMILES:	Clc1cc2c(cc1Cl)Oc1c(cc(Br)c(Br)c1Br)O2
Mol. weight [g/mol]:	489.77

Physical Properties

Property code	Value	Unit	Source
gf	134.99	kJ/mol	Joback Method
hf	-15.43	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.179		Crippen Method
mcpvol	210.280	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	896.56	K	Joback Method
tc	1187.57	K	Joback Method
tf	683.56	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.58	J/molxK	896.56	Joback Method
cpg	455.30	J/molxK	1139.07	Joback Method
cpg	447.51	J/molxK	1090.57	Joback Method
cpg	440.23	J/molxK	1042.06	Joback Method
cpg	433.27	J/molxK	993.56	Joback Method
cpg	426.45	J/molxK	945.06	Joback Method

cpg	463.77	J/molxK	1187.57	Joback Method
dvisc	0.0003460	Paxs	896.56	Joback Method
dvisc	0.0003849	Paxs	861.06	Joback Method
dvisc	0.0004321	Paxs	825.56	Joback Method
dvisc	0.0004902	Paxs	790.06	Joback Method
dvisc	0.0005628	Paxs	754.56	Joback Method
dvisc	0.0006549	Paxs	719.06	Joback Method
dvisc	0.0007743	Paxs	683.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R170680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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