Dibenzodioxin, 2,9-dibromo-, 1,3,6,8-tetrachloro-

Other names: 2,9-dibromo-1,3,6,8-tetrachloro-dibenzo-p-dioxin

Inchi: InChI=1S/C12H2Br2Cl4O2/c13-7-4(16)2-6-11(9(7)18)20-12-8(14)3(15)1-5(17)10(12)19-6

InchiKey: IQSPPDJWVNQKRB-UHFFFAOYSA-N

Formula: C12H2Br2Cl4O2

SMILES: Clc1cc2c(c(Cl)c1Br)Oc1c(Br)c(Cl)cc(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	2943.00		NIST Webbook
rinpol	2943.00		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/mol×K	910.24	Joback Method
cpg	458.74	J/mol×K	1147.64	Joback Method
cpg	451.96	J/mol×K	1100.16	Joback Method
cpg	445.52	J/mol×K	1052.68	Joback Method
cpg	439.29	J/mol×K	1005.20	Joback Method
cpg	433.11	J/mol×K	957.72	Joback Method
cpg	466.02	J/mol×K	1195.12	Joback Method

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R171950&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

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