

1,2-dibromo,4,9-dichloro-dibenzo-dioxin

Inchi:	InChI=1S/C12H4Br2Cl2O2/c13-5-4-7(16)11-12(9(5)14)18-10-6(15)2-1-3-8(10)17-11/h1-4
InchiKey:	WQLCSCDQQMTYJS-UHFFFAOYSA-N
Formula:	C12H4Br2Cl2O2
SMILES:	Clc1cccc2c1Oc1c(Br)c(Br)cc(Cl)c1O2
Mol. weight [g/mol]:	410.87

Physical Properties

Property code	Value	Unit	Source
gf	130.30	kJ/mol	Joback Method
hf	-30.29	kJ/mol	Joback Method
hfus	46.67	kJ/mol	Joback Method
hvap	81.54	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.416		Crippen Method
mcvol	192.780	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	2563.00		NIST Webbook
tb	825.42	K	Joback Method
tc	1108.05	K	Joback Method
tf	611.24	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.92	J/molxK	825.42	Joback Method
cpg	437.04	J/molxK	1060.95	Joback Method
cpg	430.15	J/molxK	1013.84	Joback Method
cpg	423.35	J/molxK	966.74	Joback Method
cpg	416.49	J/molxK	919.63	Joback Method
cpg	409.40	J/molxK	872.53	Joback Method
cpg	444.20	J/molxK	1108.05	Joback Method
dvisc	0.0004177	Paxs	825.42	Joback Method
dvisc	0.0004681	Paxs	789.72	Joback Method

dvisc	0.0005304	Paxs	754.03	Joback Method
dvisc	0.0006085	Paxs	718.33	Joback Method
dvisc	0.0007082	Paxs	682.63	Joback Method
dvisc	0.0008382	Paxs	646.94	Joback Method
dvisc	0.0010117	Paxs	611.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172433&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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