

1-bromo,2,4,6,7,9-pentachloro-dibenzo-dioxin

Inchi:	InChI=1S/C12H2BrCl5O2/c13-7-3(14)1-5(16)9-11(7)19-10-6(17)2-4(15)8(18)12(10)20-9/
InchiKey:	JYBLMFICMILPCH-UHFFFAOYSA-N
Formula:	C12H2BrCl5O2
SMILES:	Clc1cc(Cl)c2c(c1Cl)Oc1c(Cl)cc(Cl)c(Br)c1O2
Mol. weight [g/mol]:	435.31

Physical Properties

Property code	Value	Unit	Source
gf	60.93	kJ/mol	Joback Method
hf	-126.78	kJ/mol	Joback Method
hfus	53.20	kJ/mol	Joback Method
hvap	89.58	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.614		Crippen Method
mcvol	212.000	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	2772.00		NIST Webbook
rinpol	2772.00		NIST Webbook
tb	881.51	K	Joback Method
tc	1159.42	K	Joback Method
tf	666.24	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.41	J/molxK	881.51	Joback Method
cpg	452.08	J/molxK	1113.10	Joback Method
cpg	446.17	J/molxK	1066.78	Joback Method
cpg	440.37	J/molxK	1020.46	Joback Method
cpg	434.56	J/molxK	974.15	Joback Method
cpg	428.61	J/molxK	927.83	Joback Method
cpg	458.23	J/molxK	1159.42	Joback Method
dvisc	0.0003648	Paxs	881.51	Joback Method

dvisc	0.0004058	Paxs	845.63	Joback Method
dvisc	0.0004556	Paxs	809.75	Joback Method
dvisc	0.0005171	Paxs	773.88	Joback Method
dvisc	0.0005942	Paxs	738.00	Joback Method
dvisc	0.0006924	Paxs	702.12	Joback Method
dvisc	0.0008204	Paxs	666.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172646&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
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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