

6-bromo,1,2,3,4,7,9-hexachloro-dibenzo-dioxin

Inchi:	InChI=1S/C12HBrCl6O2/c13-4-2(14)1-3(15)9-10(4)21-12-8(19)6(17)5(16)7(18)11(12)20-
InchiKey:	RPHYUWFDPWLYOQ-UHFFFAOYSA-N
Formula:	C12HBrCl6O2
SMILES:	Clc1cc(Cl)c2c(c1Br)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1O2
Mol. weight [g/mol]:	469.76

Physical Properties

Property code	Value	Unit	Source
gf	39.37	kJ/mol	Joback Method
hf	-153.99	kJ/mol	Joback Method
hfus	57.01	kJ/mol	Joback Method
hvap	94.63	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	8.268		Crippen Method
mcvol	224.240	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	923.92	K	Joback Method
tc	1203.14	K	Joback Method
tf	708.68	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.87	J/molxK	923.92	Joback Method
cpg	439.53	J/molxK	970.46	Joback Method
cpg	445.05	J/molxK	1016.99	Joback Method
cpg	450.53	J/molxK	1063.53	Joback Method
cpg	456.10	J/molxK	1110.07	Joback Method
cpg	461.87	J/molxK	1156.61	Joback Method
cpg	467.95	J/molxK	1203.14	Joback Method

dvisc	0.0007039	Paxs	708.68	Joback Method
dvisc	0.0006007	Paxs	744.55	Joback Method
dvisc	0.0005202	Paxs	780.43	Joback Method
dvisc	0.0004562	Paxs	816.30	Joback Method
dvisc	0.0004046	Paxs	852.17	Joback Method
dvisc	0.0003623	Paxs	888.05	Joback Method
dvisc	0.0003272	Paxs	923.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172295&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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