

1-bromo,3,6,8-trichloro-dibenzo-dioxin

Inchi:	InChI=1S/C12H4BrCl3O2/c13-7-1-5(14)3-9-11(7)17-10-4-6(15)2-8(16)12(10)18-9/h1-4H
InchiKey:	MRJXCGJRAQRUSS-UHFFFAOYSA-N
Formula:	C12H4BrCl3O2
SMILES:	Clc1cc(Cl)c2c(c1)Oc1c(Br)cc(Cl)cc1O2
Mol. weight [g/mol]:	366.42

Physical Properties

Property code	Value	Unit	Source
gf	104.05	kJ/mol	Joback Method
hf	-72.36	kJ/mol	Joback Method
hfus	45.58	kJ/mol	Joback Method
hvap	79.49	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.307		Crippen Method
mcvol	187.520	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	796.69	K	Joback Method
tc	1071.66	K	Joback Method
tf	581.36	K	Joback Method
vc	0.709	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.46	J/molxK	796.69	Joback Method
cpg	404.13	J/molxK	842.52	Joback Method
cpg	411.28	J/molxK	888.35	Joback Method
cpg	418.04	J/molxK	934.17	Joback Method
cpg	424.55	J/molxK	980.00	Joback Method
cpg	430.95	J/molxK	1025.83	Joback Method
cpg	437.37	J/molxK	1071.66	Joback Method
dvisc	0.0011065	Paxs	581.36	Joback Method

dvisc	0.0009086	Paxs	617.25	Joback Method
dvisc	0.0007624	Paxs	653.14	Joback Method
dvisc	0.0006515	Paxs	689.03	Joback Method
dvisc	0.0005655	Paxs	724.91	Joback Method
dvisc	0.0004974	Paxs	760.80	Joback Method
dvisc	0.0004427	Paxs	796.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172666&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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