

2-bromo,1,3-dichloro-dibenzo-dioxin

Inchi:	InChI=1S/C12H5BrCl2O2/c13-10-6(14)5-9-12(11(10)15)17-8-4-2-1-3-7(8)16-9/h1-5H
InchiKey:	XBZQZPFABBXDBG-UHFFFAOYSA-N
Formula:	C12H5BrCl2O2
SMILES:	Clc1cc2c(c(Cl)c1Br)Oc1ccccc1O2
Mol. weight [g/mol]:	331.98

Physical Properties

Property code	Value	Unit	Source
gf	125.61	kJ/mol	Joback Method
hf	-45.15	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	74.44	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.654		Crippen Method
mcvol	175.280	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpola	2302.00		NIST Webbook
tb	754.28	K	Joback Method
tc	1027.42	K	Joback Method
tf	538.92	K	Joback Method
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.64	J/molxK	754.28	Joback Method
cpg	419.46	J/molxK	981.90	Joback Method
cpg	412.67	J/molxK	936.37	Joback Method
cpg	405.64	J/molxK	890.85	Joback Method
cpg	398.22	J/molxK	845.33	Joback Method
cpg	390.26	J/molxK	799.80	Joback Method
cpg	426.14	J/molxK	1027.42	Joback Method
dvisc	0.0004801	Paxs	754.28	Joback Method
dvisc	0.0005427	Paxs	718.39	Joback Method

dvisc	0.0006214	Paxs	682.49	Joback Method
dvisc	0.0007224	Paxs	646.60	Joback Method
dvisc	0.0008547	Paxs	610.71	Joback Method
dvisc	0.0010327	Paxs	574.81	Joback Method
dvisc	0.0012797	Paxs	538.92	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172804&Units=SI

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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