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

Inchi: InChI=1S/C12H5BrCl2O2/c13-6-1-2-9-10(3-6)16-11-5-7(14)4-8(15)12(11)17-9/h1-5H
InchiKey: AJVDEEVJPOHEPZ-UHFFFAOYSA-N
Formula: C12H5BrCl2O2
SMILES: Clc1cc(Cl)c2c(c1)Oc1cc(Br)ccc1O2
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
rinpol	2204.00		NIST Webbook
rinpol	2204.00		NIST Webbook
tb	754.28	K	Joback Method
tc	1027.42	K	Joback Method
tf	538.92	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.64	J/mol×K	754.28	Joback Method
cpg	390.26	J/mol×K	799.80	Joback Method
cpg	398.22	J/mol×K	845.33	Joback Method
cpg	405.64	J/mol×K	890.85	Joback Method
cpg	412.67	J/mol×K	936.37	Joback Method
cpg	419.46	J/mol×K	981.90	Joback Method
cpg	426.14	J/mol×K	1027.42	Joback Method
dvisc	0.0012797	Pa×s	538.92	Joback Method

dvisc	0.0010327	Pa×s	574.81	Joback Method
dvisc	0.0008547	Pa×s	610.71	Joback Method
dvisc	0.0007224	Pa×s	646.60	Joback Method
dvisc	0.0006214	Pa×s	682.49	Joback Method
dvisc	0.0005427	Pa×s	718.39	Joback Method
dvisc	0.0004801	Pa×s	754.28	Joback Method

Sources

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=R172908&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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