2-bromo,1-chloro-dibenzo-dioxin

Inchi: InChI=1S/C12H6BrClO2/c13-7-5-6-10-12(11(7)14)16-9-4-2-1-3-8(9)15-10/h1-6H
InchiKey: LNKMBHLFTOFOQZ-UHFFFAOYSA-N
Formula: C12H6BrClO2
SMILES: Clc1c(Br)ccc2c1Oc1ccccc1O2
Mol. weight [g/mol]: 297.53

Physical Properties

Property code	Value	Unit	Source
gf	147.17	kJ/mol	Joback Method
hf	-17.94	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	69.40	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	5.000		Crippen Method
mcvol	163.040	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	2110.00		NIST Webbook
tb	711.87	K	Joback Method
tc	982.80	K	Joback Method
tf	496.48	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.30	J/mol×K	711.87	Joback Method
cpg	375.05	J/mol×K	757.02	Joback Method
cpg	383.97	J/mol×K	802.18	Joback Method
cpg	392.21	J/mol×K	847.33	Joback Method
cpg	399.90	J/mol×K	892.49	Joback Method
cpg	407.19	J/mol×K	937.64	Joback Method
cpg	414.24	J/mol×K	982.80	Joback Method
dvisc	0.0014752	Pa×s	496.48	Joback Method
dvisc	0.0011662	Pa×s	532.38	Joback Method

dvisc	0.0009497	Pa×s	568.28	Joback Method
dvisc	0.0007925	Pa×s	604.17	Joback Method
dvisc	0.0006749	Pa×s	640.07	Joback Method
dvisc	0.0005847	Pa×s	675.97	Joback Method
dvisc	0.0005139	Pa×s	711.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R172839&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