2,3-dibromo-7-chlorodibenzo-p-dioxin

Inchi: InChI=1S/C12H5Br2ClO2/c13-7-4-11-12(5-8(7)14)17-10-3-6(15)1-2-9(10)16-11/h1-5H
InchiKey: SSBCMPITQJYXFS-UHFFFAOYSA-N
Formula: C12H5Br2ClO2
SMILES: Clc1ccc2c(c1)Oc1cc(Br)c(Br)cc1O2
Mol. weight [g/mol]: 376.43

Physical Properties

Property code	Value	Unit	Source
gf	151.86	kJ/mol	Joback Method
hf	-3.08	kJ/mol	Joback Method
hfus	42.86	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.763		Crippen Method
mcvol	180.540	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
rinpol	2375.00		NIST Webbook
tb	783.01	K	Joback Method
tc	1064.23	K	Joback Method
tf	568.80	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.83	J/mol×K	783.01	Joback Method
cpg	396.16	J/mol×K	829.88	Joback Method
cpg	403.93	J/mol×K	876.75	Joback Method
cpg	411.31	J/mol×K	923.62	Joback Method
cpg	418.46	J/mol×K	970.49	Joback Method
cpg	425.55	J/mol×K	1017.36	Joback Method
cpg	432.77	J/mol×K	1064.23	Joback Method
dvisc	0.0011822	Pa×s	568.80	Joback Method
dvisc	0.0009641	Pa×s	604.50	Joback Method

dvisc	0.0008043	Pa×s	640.20	Joback Method
dvisc	0.0006840	Pa×s	675.90	Joback Method
dvisc	0.0005912	Pa×s	711.61	Joback Method
dvisc	0.0005182	Pa×s	747.31	Joback Method
dvisc	0.0004597	Pa×s	783.01	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=R171821&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