Dibenzo-p-dioxin, 1,3-dichloro-

Inchi: InChI=1S/C12H6Cl2O2/c13-7-5-8(14)12-11(6-7)15-9-3-1-2-4-10(9)16-12/h1-6H
InchiKey: AZYJYMAKTBXNSX-UHFFFAOYSA-N
Formula: C12H6Cl2O2
SMILES: Clc1cc(Cl)c2c(c1)Oc1ccccc1O2
Mol. weight [g/mol]: 253.08
CAS: 50585-39-2

Physical Properties

Property code	Value	Unit	Source
gf	120.92	kJ/mol	Joback Method
hf	-60.01	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.891		Crippen Method
mcvol	157.780	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	683.14	K	Joback Method
tc	945.37	K	Joback Method
tf	466.60	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.63	J/mol×K	683.14	Joback Method
cpg	367.82	J/mol×K	726.84	Joback Method
cpg	377.11	J/mol×K	770.55	Joback Method
cpg	385.63	J/mol×K	814.25	Joback Method
cpg	393.51	J/mol×K	857.96	Joback Method
cpg	400.86	J/mol×K	901.66	Joback Method

cpg	407.80	J/mol×K	945.37	Joback Method
dvisc	0.0015388	Pa×s	466.60	Joback Method
dvisc	0.0011999	Pa×s	502.69	Joback Method
dvisc	0.0009673	Pa×s	538.78	Joback Method
dvisc	0.0008012	Pa×s	574.87	Joback Method
dvisc	0.0006785	Pa×s	610.96	Joback Method
dvisc	0.0005854	Pa×s	647.05	Joback Method
dvisc	0.0005130	Pa×s	683.14	Joback Method

Sources

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=C50585392&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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