Dibenzo-p-dioxin, 1,2,7-trichloro

Inchi: InChI=1S/C12H5Cl3O2/c13-6-1-3-8-10(5-6)16-9-4-2-7(14)11(15)12(9)17-8/h1-5H
InchiKey: TXJMXDWFPQSYEQ-UHFFFAOYSA-N
Formula: C12H5Cl3O2
SMILES: Clc1ccc2c(c1)Oc1ccc(Cl)c(Cl)c1O2
Mol. weight [g/mol]: 287.53

Physical Properties

Property code	Value	Unit	Source
gf	99.36	kJ/mol	Joback Method
hf	-87.22	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	72.39	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	5.545		Crippen Method
mcvol	170.020	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2192.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	725.55	K	Joback Method
tc	990.47	K	Joback Method
tf	509.04	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.96	J/mol×K	725.55	Joback Method
cpg	383.94	J/mol×K	769.70	Joback Method
cpg	392.18	J/mol×K	813.86	Joback Method
cpg	399.78	J/mol×K	858.01	Joback Method
cpg	406.87	J/mol×K	902.16	Joback Method

cpg	413.56	J/mol×K	946.32	Joback Method
cpg	419.96	J/mol×K	990.47	Joback Method
dvisc	0.0013574	Pa×s	509.04	Joback Method
dvisc	0.0010829	Pa×s	545.13	Joback Method
dvisc	0.0008885	Pa×s	581.21	Joback Method
dvisc	0.0007461	Pa×s	617.30	Joback Method
dvisc	0.0006387	Pa×s	653.38	Joback Method
dvisc	0.0005557	Pa×s	689.47	Joback Method
dvisc	0.0004903	Pa×s	725.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50252&Units=SI
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

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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