

Dibenzo-p-dioxin, 2,3,7-trichloro-

Other names:	2,3,7-Trichlorodibenzo-p-dioxin 2,3,7-trichlorodibenzodioxin
Inchi:	InChI=1S/C12H5Cl3O2/c13-6-1-2-9-10(3-6)17-12-5-8(15)7(14)4-11(12)16-9/h1-5H
InchiKey:	ZSIZNEVHVVRPFF-UHFFFAOYSA-N
Formula:	C12H5Cl3O2
SMILES:	Clc1ccc2c(c1)Oc1cc(Cl)c(Cl)cc1O2
Mol. weight [g/mol]:	287.53
CAS:	33857-28-2

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	2181.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2160.00		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

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=C33857282&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

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