

8-methyl-2,3,7-trichlorodibenzodioxin

Inchi:	InChI=1S/C13H7Cl3O2/c1-6-2-10-11(3-7(6)14)18-13-5-9(16)8(15)4-12(13)17-10/h2-5H,1
InchiKey:	XUOCRPPPSAFJCF-UHFFFAOYSA-N
Formula:	C13H7Cl3O2
SMILES:	Cc1cc2c(cc1Cl)Oc1cc(Cl)c(Cl)cc1O2
Mol. weight [g/mol]:	301.55

Physical Properties

Property code	Value	Unit	Source
gf	98.15	kJ/mol	Joback Method
hf	-119.33	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.853		Crippen Method
mcvol	184.110	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	753.41	K	Joback Method
tc	1012.85	K	Joback Method
tf	532.83	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.49	J/molxK	753.41	Joback Method
cpg	432.19	J/molxK	796.65	Joback Method
cpg	441.17	J/molxK	839.89	Joback Method
cpg	449.53	J/molxK	883.13	Joback Method
cpg	457.38	J/molxK	926.37	Joback Method
cpg	464.83	J/molxK	969.61	Joback Method
cpg	471.96	J/molxK	1012.85	Joback Method
dvisc	0.0011928	Paxs	532.83	Joback Method

dvisc	0.0009615	Paxs	569.59	Joback Method
dvisc	0.0007955	Paxs	606.36	Joback Method
dvisc	0.0006726	Paxs	643.12	Joback Method
dvisc	0.0005791	Paxs	679.88	Joback Method
dvisc	0.0005064	Paxs	716.65	Joback Method
dvisc	0.0004486	Paxs	753.41	Joback Method

Sources

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=R173441&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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