

1,2-Dimethyltetrakis(chloromethyl)benzene

Inchi:	InChI=1S/C12H14Cl4/c1-7-8(2)10(4-14)12(6-16)11(5-15)9(7)3-13/h3-6H2,1-2H3
InchiKey:	ADXOBQMLRXKOA-UHFFFAOYSA-N
Formula:	C12H14Cl4
SMILES:	Cc1c(C)c(CCl)c(CCl)c(CCl)c1CCl
Mol. weight [g/mol]:	300.05

Physical Properties

Property code	Value	Unit	Source
gf	66.70	kJ/mol	Joback Method
hf	-174.79	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.259		Crippen Method
mcvol	205.140	ml/mol	McGowan Method
pc	1954.41	kPa	Joback Method
rinpol	2198.00		NIST Webbook
rinpol	2198.00		NIST Webbook
tb	675.26	K	Joback Method
tc	895.74	K	Joback Method
tf	433.70	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.44	J/molxK	675.26	Joback Method
cpg	465.56	J/molxK	712.01	Joback Method
cpg	476.97	J/molxK	748.75	Joback Method
cpg	487.70	J/molxK	785.50	Joback Method
cpg	497.76	J/molxK	822.25	Joback Method
cpg	507.19	J/molxK	859.00	Joback Method
cpg	515.99	J/molxK	895.74	Joback Method
dvisc	0.0008017	Paxs	433.70	Joback Method

dvisc	0.0005523	Paxs	473.96	Joback Method
dvisc	0.0004033	Paxs	514.22	Joback Method
dvisc	0.0003083	Paxs	554.48	Joback Method
dvisc	0.0002444	Paxs	594.74	Joback Method
dvisc	0.0001995	Paxs	635.00	Joback Method
dvisc	0.0001669	Paxs	675.26	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=R520228&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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