

2,2',4,4'-tetrachloro-5-methyl-diphenylmethane

Other names:	2,2',4,4'-tetrachlorobenzyl 5-toluene
Inchi:	InChI=1S/C14H10Cl4/c1-8-4-10(14(18)7-12(8)16)5-9-2-3-11(15)6-13(9)17/h2-4,6-7H,5H2
InchiKey:	DLJAEIAZPTWSB-UHFFFAOYSA-N
Formula:	C14H10Cl4
SMILES:	Cc1cc(Cc2ccc(Cl)cc2Cl)c(Cl)cc1Cl
Mol. weight [g/mol]:	320.04

Physical Properties

Property code	Value	Unit	Source
gf	195.95	kJ/mol	Joback Method
hf	20.46	kJ/mol	Joback Method
hfus	34.94	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-7.49		Aqueous Solubility Prediction Method
logp	6.199		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2149.10		NIST Webbook
rinpol	2149.10		NIST Webbook
rinpol	2159.80		NIST Webbook
tb	747.70	K	Joback Method
tc	1002.50	K	Joback Method
tf	482.66	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.32	J/molxK	747.70	Joback Method
cpg	477.97	J/molxK	790.17	Joback Method
cpg	488.65	J/molxK	832.63	Joback Method
cpg	498.43	J/molxK	875.10	Joback Method
cpg	507.35	J/molxK	917.56	Joback Method

cpg	515.47	J/molxK	960.03	Joback Method
cpg	522.84	J/molxK	1002.50	Joback Method
dvisc	0.0006543	Paxs	482.66	Joback Method
dvisc	0.0004524	Paxs	526.83	Joback Method
dvisc	0.0003312	Paxs	571.01	Joback Method
dvisc	0.0002535	Paxs	615.18	Joback Method
dvisc	0.0002012	Paxs	659.35	Joback Method
dvisc	0.0001643	Paxs	703.53	Joback Method
dvisc	0.0001375	Paxs	747.70	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R181150&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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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