

2,2',4,6'-tetrachloro-3-methyl-diphenylmethane

Other names:	2,2',4,6'-tetrachlorobenzyl 3-toluene
Inchi:	InChI=1S/C14H10Cl4/c1-8-11(15)6-5-9(14(8)18)7-10-12(16)3-2-4-13(10)17/h2-6H,7H2,1
InchiKey:	WQCFXZHBWZFDAX-UHFFFAOYSA-N
Formula:	C14H10Cl4
SMILES:	Cc1c(Cl)ccc(Cc2c(Cl)cccc2Cl)c1Cl
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	-7.99		Aqueous Solubility Prediction Method
logp	6.199		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2165.60		NIST Webbook
rinpol	2153.50		NIST Webbook
rinpol	2153.50		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/mol×K	747.70	Joback Method
cpg	477.97	J/mol×K	790.17	Joback Method
cpg	488.65	J/mol×K	832.63	Joback Method
cpg	498.43	J/mol×K	875.10	Joback Method
cpg	507.35	J/mol×K	917.56	Joback Method

cpg	515.47	J/mol×K	960.03	Joback Method
cpg	522.84	J/mol×K	1002.50	Joback Method
dvisc	0.0006543	Pa×s	482.66	Joback Method
dvisc	0.0004524	Pa×s	526.83	Joback Method
dvisc	0.0003312	Pa×s	571.01	Joback Method
dvisc	0.0002535	Pa×s	615.18	Joback Method
dvisc	0.0002012	Pa×s	659.35	Joback Method
dvisc	0.0001643	Pa×s	703.53	Joback Method
dvisc	0.0001375	Pa×s	747.70	Joback Method

Sources

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R181170&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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