2,2',4,6'-tetrachloro-5-methyl-diphenylmethane

Other names: 2,2',4,6'-tetrachlorobenzyl 5-toluene
Inchi: InChI=1S/C14H10Cl4/c1-8-5-9(14(18)7-13(8)17)6-10-11(15)3-2-4-12(10)16/h2-5,7H,6H2
InchiKey: LWTZRUALFAUJAX-UHFFFAOYSA-N
Formula: C14H10Cl4
SMILES: Cc1cc(Cc2c(Cl)cccc2Cl)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	-8.36		Aqueous Solubility Prediction Method
logp	6.199		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
rinpol	2102.50		NIST Webbook
rinpol	2113.30		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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R181185&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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