4-Methylbenzoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H8Cl4O2/c1-7-2-4-8(5-3-7)14(19)20-13-10(16)6-9(15)11(17)12(13)18/h2-6

InchiKey: SFJHLPXLDGAAAK-UHFFFAOYSA-N

Formula: C14H8Cl4O2

SMILES: Cc1ccc(C(=O)Oc2c(Cl)cc(Cl)c(Cl)c2Cl)cc1

Mol. weight [g/mol]: 350.02

Physical Properties

Property code	Value	Unit	Source
gf	-37.97	kJ/mol	Joback Method
hf	-224.34	kJ/mol	Joback Method
hfus	37.73	kJ/mol	Joback Method
hvap	81.32	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.828		Crippen Method
mcvol	217.000	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	2484.00		NIST Webbook
rinpol	2484.00		NIST Webbook
tb	823.99	K	Joback Method
tc	1078.98	K	Joback Method
tf	554.82	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.61	J/mol×K	823.99	Joback Method
cpg	506.20	J/mol×K	866.49	Joback Method
cpg	514.79	J/mol×K	908.99	Joback Method
cpg	522.41	J/mol×K	951.48	Joback Method
cpg	529.08	J/mol×K	993.98	Joback Method
cpg	534.83	J/mol×K	1036.48	Joback Method
cpg	539.67	J/mol×K	1078.98	Joback Method
dvisc	0.0004583	Pa×s	554.82	Joback Method

dvisc	0.0003275	Pa×s	599.68	Joback Method
dvisc	0.0002452	Pa×s	644.54	Joback Method
dvisc	0.0001906	Pa×s	689.40	Joback Method
dvisc	0.0001528	Pa×s	734.27	Joback Method
dvisc	0.0001257	Pa×s	779.13	Joback Method
dvisc	0.0001056	Pa×s	823.99	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=U354158&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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