m-Toluic acid, 4-chlorophenyl ester

Other names: m-Toluylic acid, 4-chlorophenyl ester
Inchi: InChI=1S/C14H11ClO2/c1-10-3-2-4-11(9-10)14(16)17-13-7-5-12(15)6-8-13/h2-9H,1H3
InchiKey: AFMWNHRHTYUYLU-UHFFFAOYSA-N
Formula: C14H11ClO2
SMILES: Cc1cccc(C(=O)Oc2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 246.69

Physical Properties

Property code	Value	Unit	Source
gf	26.71	kJ/mol	Joback Method
hf	-142.71	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	3.868		Crippen Method
mcvol	180.280	ml/mol	McGowan Method
pc	2709.85	kPa	Joback Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
tb	696.76	K	Joback Method
tc	943.81	K	Joback Method
tf	427.50	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.48	J/mol×K	696.76	Joback Method
cpg	452.11	J/mol×K	737.94	Joback Method
cpg	464.61	J/mol×K	779.11	Joback Method
cpg	476.03	J/mol×K	820.29	Joback Method
cpg	486.41	J/mol×K	861.46	Joback Method
cpg	495.79	J/mol×K	902.64	Joback Method
cpg	504.22	J/mol×K	943.81	Joback Method

dvisc	0.0009660	Pa×s	427.50	Joback Method
dvisc	0.0006014	Pa×s	472.38	Joback Method
dvisc	0.0004065	Pa×s	517.25	Joback Method
dvisc	0.0002925	Pa×s	562.13	Joback Method
dvisc	0.0002210	Pa×s	607.01	Joback Method
dvisc	0.0001735	Pa×s	651.88	Joback Method
dvisc	0.0001405	Pa×s	696.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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