m-Toluic acid, 3,4-dichlorophenyl ester

Other names: m-Toluylic acid, 3,4-dichlorophenyl ester
Inchi: InChI=1S/C14H10Cl2O2/c1-9-3-2-4-10(7-9)14(17)18-11-5-6-12(15)13(16)8-11/h2-8H,1H
InchiKey: YVULESXWFJKJNZ-UHFFFAOYSA-N
Formula: C14H10Cl2O2
SMILES: Cc1cccc(C(=O)Oc2ccc(Cl)c(Cl)c2)c1
Mol. weight [g/mol]: 281.13

Physical Properties

Property code	Value	Unit	Source
gf	5.15	kJ/mol	Joback Method
hf	-169.92	kJ/mol	Joback Method
hfus	30.11	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.521		Crippen Method
mcvol	192.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	739.17	K	Joback Method
tc	989.16	K	Joback Method
tf	469.94	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.79	J/mol×K	739.17	Joback Method
cpg	472.01	J/mol×K	780.84	Joback Method
cpg	483.16	J/mol×K	822.50	Joback Method
cpg	493.27	J/mol×K	864.17	Joback Method
cpg	502.38	J/mol×K	905.83	Joback Method
cpg	510.53	J/mol×K	947.50	Joback Method
cpg	517.76	J/mol×K	989.16	Joback Method

dvisc	0.0007416	Pa×s	469.94	Joback Method
dvisc	0.0004884	Pa×s	514.81	Joback Method
dvisc	0.0003439	Pa×s	559.68	Joback Method
dvisc	0.0002551	Pa×s	604.56	Joback Method
dvisc	0.0001972	Pa×s	649.43	Joback Method
dvisc	0.0001576	Pa×s	694.30	Joback Method
dvisc	0.0001294	Pa×s	739.17	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=U307570&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