m-Toluic acid, 3,5-dimethylphenyl ester

Other names: m-Toluylic acid, 3,5-dimethylphenyl ester
Inchi: InChI=1S/C16H16O2/c1-11-5-4-6-14(8-11)16(17)18-15-9-12(2)7-13(3)10-15/h4-10H,1-3H
InchiKey: KOXGVGQBHWUCCS-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: Cc1cc(C)cc(OC(=O)c2cccc(C)c2)c1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	45.85	kJ/mol	Joback Method
hf	-179.72	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.831		Crippen Method
mcvol	196.220	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	710.07	K	Joback Method
tc	945.48	K	Joback Method
tf	432.64	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.08	J/mol×K	710.07	Joback Method
cpg	531.74	J/mol×K	749.31	Joback Method
cpg	546.25	J/mol×K	788.54	Joback Method
cpg	559.64	J/mol×K	827.78	Joback Method
cpg	571.96	J/mol×K	867.01	Joback Method
cpg	583.23	J/mol×K	906.25	Joback Method
cpg	593.49	J/mol×K	945.48	Joback Method

dvisc	0.0008112	Pa×s	432.64	Joback Method
dvisc	0.0005079	Pa×s	478.88	Joback Method
dvisc	0.0003453	Pa×s	525.12	Joback Method
dvisc	0.0002499	Pa×s	571.36	Joback Method
dvisc	0.0001898	Pa×s	617.59	Joback Method
dvisc	0.0001498	Pa×s	663.83	Joback Method
dvisc	0.0001219	Pa×s	710.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307567&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