m-Toluic acid, pentyl ester

Other names: m-Toluylic acid, pentyl ester
Inchi: InChI=1S/C13H18O2/c1-3-4-5-9-15-13(14)12-8-6-7-11(2)10-12/h6-8,10H,3-5,9H2,1-2H3
InchiKey: KUPGUGAJEZQRKM-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCCCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 206.28
CAS: 5448-60-2

Physical Properties

Property code	Value	Unit	Source
gf	-72.56	kJ/mol	Joback Method
hf	-331.39	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	56.63	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.342		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
rinpol	1610.90		NIST Webbook
tb	604.79	K	Joback Method
tc	808.65	K	Joback Method
tf	347.37	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.04	J/mol×K	604.79	Joback Method
cpg	512.69	J/mol×K	774.67	Joback Method
cpg	500.37	J/mol×K	740.70	Joback Method
cpg	487.26	J/mol×K	706.72	Joback Method
cpg	473.35	J/mol×K	672.74	Joback Method
cpg	458.61	J/mol×K	638.77	Joback Method
cpg	524.25	J/mol×K	808.65	Joback Method

dvisc	0.0001649	Pa×s	604.79	Joback Method
dvisc	0.0002092	Pa×s	561.89	Joback Method
dvisc	0.0002761	Pa×s	518.98	Joback Method
dvisc	0.0003830	Pa×s	476.08	Joback Method
dvisc	0.0005669	Pa×s	433.18	Joback Method
dvisc	0.0009147	Pa×s	390.27	Joback Method
dvisc	0.0016609	Pa×s	347.37	Joback Method

Sources

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=C5448602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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