o-Toluic acid, pentyl ester

Other names: o-Toluylic acid, pentyl ester
Inchi: InChI=1S/C13H18O2/c1-3-4-7-10-15-13(14)12-9-6-5-8-11(12)2/h5-6,8-9H,3-4,7,10H2,1-2
InchiKey: YMAHRBGBVUOIMQ-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]: 206.28
CAS: 65382-89-0

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	1569.00		NIST Webbook
rinpol	1569.00		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	458.61	J/mol×K	638.77	Joback Method
cpg	473.35	J/mol×K	672.74	Joback Method
cpg	487.26	J/mol×K	706.72	Joback Method
cpg	500.37	J/mol×K	740.70	Joback Method
cpg	512.69	J/mol×K	774.67	Joback Method

cpg	524.25	J/mol×K	808.65	Joback Method
dvisc	0.0016609	Pa×s	347.37	Joback Method
dvisc	0.0009147	Pa×s	390.27	Joback Method
dvisc	0.0005669	Pa×s	433.18	Joback Method
dvisc	0.0003830	Pa×s	476.08	Joback Method
dvisc	0.0002761	Pa×s	518.98	Joback Method
dvisc	0.0002092	Pa×s	561.89	Joback Method
dvisc	0.0001649	Pa×s	604.79	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65382890&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

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

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