p-Toluylic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H14O2/c1-11-6-8-13(9-7-11)15(16)17-14-5-3-4-12(2)10-14/h3-10H,1-2H3
InchiKey: YOLXLRZYVQUCIC-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: Cc1ccc(C(=O)Oc2cccc(C)c2)cc1
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	47.06	kJ/mol	Joback Method
hf	-147.61	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	64.02	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.523		Crippen Method
mcvol	182.130	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1874.00		NIST Webbook
tb	682.21	K	Joback Method
tc	921.60	K	Joback Method
tf	408.85	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.87	J/mol×K	682.21	Joback Method
cpg	530.68	J/mol×K	881.70	Joback Method
cpg	519.68	J/mol×K	841.80	Joback Method
cpg	507.64	J/mol×K	801.91	Joback Method
cpg	494.51	J/mol×K	762.01	Joback Method
cpg	480.27	J/mol×K	722.11	Joback Method
cpg	540.68	J/mol×K	921.60	Joback Method
dvisc	0.0001351	Pa×s	682.21	Joback Method
dvisc	0.0001676	Pa×s	636.65	Joback Method

dvisc	0.0002150	Pa×s	591.09	Joback Method
dvisc	0.0002874	Pa×s	545.53	Joback Method
dvisc	0.0004052	Pa×s	499.97	Joback Method
dvisc	0.0006119	Pa×s	454.41	Joback Method
dvisc	0.0010130	Pa×s	408.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307764&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