p-Toluic acid, 2-methylphenyl ester

Other names: 2-Methylphenyl 4-methylbenzoate
p-Toluylic acid, 2-methylphenyl ester
Inchi: InChI=1S/C15H14O2/c1-11-7-9-13(10-8-11)15(16)17-14-6-4-3-5-12(14)2/h3-10H,1-2H3
InchiKey: IEKFWPTVAIWBBX-UHFFFAOYSA-N
Formula: C15H14O2
SMILES: Cc1ccc(C(=O)Oc2ccccc2C)cc1
Mol. weight [g/mol]: 226.27
CAS: 23597-29-7

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	1832.90		NIST Webbook
rinpol	1832.90		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	480.27	J/mol×K	722.11	Joback Method
cpg	494.51	J/mol×K	762.01	Joback Method
cpg	507.64	J/mol×K	801.91	Joback Method
cpg	519.68	J/mol×K	841.80	Joback Method

cpg	530.68	J/mol×K	881.70	Joback Method
cpg	540.68	J/mol×K	921.60	Joback Method
dvisc	0.0010130	Pa×s	408.85	Joback Method
dvisc	0.0006119	Pa×s	454.41	Joback Method
dvisc	0.0004052	Pa×s	499.97	Joback Method
dvisc	0.0002874	Pa×s	545.53	Joback Method
dvisc	0.0002150	Pa×s	591.09	Joback Method
dvisc	0.0001676	Pa×s	636.65	Joback Method
dvisc	0.0001351	Pa×s	682.21	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23597297&Units=SI

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