m-Toluic acid, hexyl ester

Other names: m-Toluylic acid, hexyl ester
Hexyl 3-methylbenzoate
Inchi: InChI=1S/C14H20O2/c1-3-4-5-6-10-16-14(15)13-9-7-8-12(2)11-13/h7-9,11H,3-6,10H2,1-
InchiKey: GYAMMOVKXUZHFX-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 220.31
CAS: 67101-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-64.14	kJ/mol	Joback Method
hf	-352.03	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.732		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1707.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1707.00		NIST Webbook
tb	627.67	K	Joback Method
tc	828.65	K	Joback Method
tf	358.64	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.85	J/mol×K	627.67	Joback Method
cpg	509.98	J/mol×K	661.17	Joback Method
cpg	525.23	J/mol×K	694.66	Joback Method

cpg	539.64	J/mol×K	728.16	Joback Method
cpg	553.21	J/mol×K	761.65	Joback Method
cpg	565.96	J/mol×K	795.15	Joback Method
cpg	577.93	J/mol×K	828.65	Joback Method
dvisc	0.0015939	Pa×s	358.64	Joback Method
dvisc	0.0008632	Pa×s	403.48	Joback Method
dvisc	0.0005285	Pa×s	448.32	Joback Method
dvisc	0.0003538	Pa×s	493.16	Joback Method
dvisc	0.0002532	Pa×s	537.99	Joback Method
dvisc	0.0001908	Pa×s	582.83	Joback Method
dvisc	0.0001497	Pa×s	627.67	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=C67101637&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