m-Toluic acid, octyl ester

Other names: m-Toluylic acid, octyl ester
Inchi: InChI=1S/C16H24O2/c1-3-4-5-6-7-8-12-18-16(17)15-11-9-10-14(2)13-15/h9-11,13H,3-8,
InchiKey: HGEOTNHWCJQOTI-UHFFFAOYSA-N
Formula: C16H24O2
SMILES: CCCCCCCCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 248.36
CAS: 16409-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-47.30	kJ/mol	Joback Method
hf	-393.31	kJ/mol	Joback Method
hfus	33.63	kJ/mol	Joback Method
hvap	63.30	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.512		Crippen Method
mcvol	219.980	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	673.43	K	Joback Method
tc	869.56	K	Joback Method
tf	381.18	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.73	J/mol×K	673.43	Joback Method
cpg	616.73	J/mol×K	706.12	Joback Method
cpg	632.81	J/mol×K	738.81	Joback Method
cpg	647.97	J/mol×K	771.49	Joback Method
cpg	662.26	J/mol×K	804.18	Joback Method
cpg	675.69	J/mol×K	836.87	Joback Method

cpg	688.29	J/mol×K	869.56	Joback Method
dvisc	0.0014273	Pa×s	381.18	Joback Method
dvisc	0.0007494	Pa×s	429.89	Joback Method
dvisc	0.0004486	Pa×s	478.60	Joback Method
dvisc	0.0002953	Pa×s	527.31	Joback Method
dvisc	0.0002086	Pa×s	576.01	Joback Method
dvisc	0.0001555	Pa×s	624.72	Joback Method
dvisc	0.0001210	Pa×s	673.43	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16409248&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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