o-Toluic acid, decyl ester

Other names: o-Toluylic acid, decyl ester
Inchi: InChI=1S/C18H28O2/c1-3-4-5-6-7-8-9-12-15-20-18(19)17-14-11-10-13-16(17)2/h10-11,1
InchiKey: JTRXLGJPZKNYRY-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]: 276.41
CAS: 107141-17-3

Physical Properties

Property code	Value	Unit	Source
gf	-30.46	kJ/mol	Joback Method
hf	-434.59	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.293		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2082.20		NIST Webbook
rinpol	2082.20		NIST Webbook
tb	719.19	K	Joback Method
tc	912.00	K	Joback Method
tf	403.72	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.68	J/mol×K	719.19	Joback Method
cpg	728.33	J/mol×K	751.33	Joback Method
cpg	745.01	J/mol×K	783.46	Joback Method
cpg	760.73	J/mol×K	815.60	Joback Method
cpg	775.53	J/mol×K	847.73	Joback Method
cpg	789.43	J/mol×K	879.87	Joback Method

cpg	802.46	J/mol×K	912.00	Joback Method
dvisc	0.0012384	Pa×s	403.72	Joback Method
dvisc	0.0006322	Pa×s	456.30	Joback Method
dvisc	0.0003708	Pa×s	508.88	Joback Method
dvisc	0.0002404	Pa×s	561.46	Joback Method
dvisc	0.0001678	Pa×s	614.03	Joback Method
dvisc	0.0001240	Pa×s	666.61	Joback Method
dvisc	0.0000958	Pa×s	719.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107141173&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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