o-Toluic acid, nonyl ester

Other names:	o-Toluylic acid, nonyl ester
	Benzoic acid, 2-methyl-, nonyl ester
Inchi:	InChI=1S/C17H26O2/c1-3-4-5-6-7-8-11-14-19-17(18)16-13-10-9-12-15(16)2/h9-10,12-13
InchiKey:	SQNNJZFKCWXFBT-UHFFFAOYSA-N
Formula:	C17H26O2
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	262.39
CAS:	343598-14-1

Physical Properties

Property code	Value	Unit	Source
gf	-38.88	kJ/mol	Joback Method
hf	-413.95	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.902		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	1965.70		NIST Webbook
tb	696.31	K	Joback Method
tc	890.56	K	Joback Method
tf	392.45	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.61	J/mol×K	696.31	Joback Method
cpg	671.96	J/mol×K	728.69	Joback Method
cpg	688.36	J/mol×K	761.06	Joback Method
cpg	703.83	J/mol×K	793.44	Joback Method
cpg	718.39	J/mol×K	825.81	Joback Method
cpg	732.07	J/mol×K	858.19	Joback Method

cpg	744.91	J/mol×K	890.56	Joback Method
dvisc	0.0013343	Pa×s	392.45	Joback Method
dvisc	0.0006905	Pa×s	443.09	Joback Method
dvisc	0.0004091	Pa×s	493.74	Joback Method
dvisc	0.0002671	Pa×s	544.38	Joback Method
dvisc	0.0001876	Pa×s	595.02	Joback Method
dvisc	0.0001392	Pa×s	645.67	Joback Method
dvisc	0.0001079	Pa×s	696.31	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=C343598141&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

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