

p-Toluic acid, nonyl ester

Other names:	p-toluylic acid, nonyl ester
Inchi:	InChI=1S/C17H26O2/c1-3-4-5-6-7-8-9-14-19-17(18)16-12-10-15(2)11-13-16/h10-13H,3-9
InchiKey:	KKKOQJXGARKBNU-UHFFFAOYSA-N
Formula:	C17H26O2
SMILES:	CCCCCCCCCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	262.39

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
mvol	234.070	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
rinpol	2015.10		NIST Webbook
rinpol	2015.10		NIST Webbook
tb	696.31	K	Joback Method
tc	890.56	K	Joback Method
tf	392.45	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.61	J/mol×K	696.31	Joback Method
cpg	732.07	J/mol×K	858.19	Joback Method
cpg	718.39	J/mol×K	825.81	Joback Method
cpg	703.83	J/mol×K	793.44	Joback Method
cpg	688.36	J/mol×K	761.06	Joback Method
cpg	671.96	J/mol×K	728.69	Joback Method
cpg	744.91	J/mol×K	890.56	Joback Method

dvisc	0.0001079	Paxs	696.31	Joback Method
dvisc	0.0001392	Paxs	645.67	Joback Method
dvisc	0.0001876	Paxs	595.02	Joback Method
dvisc	0.0002671	Paxs	544.38	Joback Method
dvisc	0.0004091	Paxs	493.74	Joback Method
dvisc	0.0006905	Paxs	443.09	Joback Method
dvisc	0.0013343	Paxs	392.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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