p-Toluic acid, undec-2-enyl ester

Other names: p-toluylic acid, undec-2-enyl ester
Inchi: InChI=1S/C19H28O2/c1-3-4-5-6-7-8-9-10-11-16-21-19(20)18-14-12-17(2)13-15-18/h10-1
InchiKey: LPDKAMRSUALKNB-ZHACJKMWSA-N
Formula: C19H28O2
SMILES: CCCCCCCCC=CCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 288.42

Physical Properties

Property code	Value	Unit	Source
gf	58.18	kJ/mol	Joback Method
hf	-338.01	kJ/mol	Joback Method
hfus	41.61	kJ/mol	Joback Method
hvap	69.94	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.459		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2237.70		NIST Webbook
rinpol	2237.70		NIST Webbook
tb	746.23	K	Joback Method
tc	943.58	K	Joback Method
tf	409.91	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.01	J/mol×K	746.23	Joback Method
cpg	761.47	J/mol×K	779.12	Joback Method
cpg	777.94	J/mol×K	812.01	Joback Method
cpg	793.45	J/mol×K	844.90	Joback Method
cpg	808.04	J/mol×K	877.79	Joback Method
cpg	821.75	J/mol×K	910.69	Joback Method
cpg	834.64	J/mol×K	943.58	Joback Method

dvisc	0.0010565	Pa×s	409.91	Joback Method
dvisc	0.0005184	Pa×s	465.96	Joback Method
dvisc	0.0002964	Pa×s	522.02	Joback Method
dvisc	0.0001889	Pa×s	578.07	Joback Method
dvisc	0.0001303	Pa×s	634.12	Joback Method
dvisc	0.0000955	Pa×s	690.18	Joback Method
dvisc	0.0000733	Pa×s	746.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292508&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