O-toluic acid, 2-tridecyl ester

Other names: o-Toluylic acid, 2-tridecyl ester
Inchi: InChI=1S/C21H34O2/c1-4-5-6-7-8-9-10-11-12-16-19(3)23-21(22)20-17-14-13-15-18(20)2
InchiKey: YCVBLJATVOWYST-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: CCCCCCCCCCCC(C)OC(=O)c1ccccc1C
Mol. weight [g/mol]: 318.50

Physical Properties

Property code	Value	Unit	Source
hf	-570.20	kJ/mol	Cheméo Relay (1.0)
hfus	43.06	kJ/mol	Joback Method
hvap	101.40	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-6.45		Cheméo Relay (1.0)
logp	6.461		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
tb	612.98	K	Cheméo Relay (1.0)
tf	276.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.66	J/mol×K	787.39	Joback Method
cpg	904.28	J/mol×K	819.64	Joback Method
cpg	921.80	J/mol×K	851.89	Joback Method
cpg	938.27	J/mol×K	884.13	Joback Method
cpg	953.71	J/mol×K	916.38	Joback Method
cpg	968.16	J/mol×K	948.63	Joback Method
cpg	981.66	J/mol×K	980.88	Joback Method
dvisc	0.0011307	Pa×s	422.53	Joback Method
dvisc	0.0005097	Pa×s	483.34	Joback Method

dvisc	0.0002745	Pa×s	544.15	Joback Method
dvisc	0.0001674	Pa×s	604.96	Joback Method
dvisc	0.0001118	Pa×s	665.77	Joback Method
dvisc	0.0000799	Pa×s	726.58	Joback Method
dvisc	0.0000601	Pa×s	787.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299790&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point