O-toluic acid, 4-tetradecyl ester

Other names: o-Toluylic acid, 4-tetradecyl ester
Inchi: InChI=1S/C22H36O2/c1-4-6-7-8-9-10-11-12-17-20(15-5-2)24-22(23)21-18-14-13-16-19(2
InchiKey: LAMMNLIWBMGULQ-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCC(CCC)OC(=O)c1ccccc1C
Mol. weight [g/mol]: 332.53

Physical Properties

Property code	Value	Unit	Source
hf	-575.62	kJ/mol	Cheméo Relay (1.0)
hfus	45.65	kJ/mol	Joback Method
hvap	104.88	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-6.78		Cheméo Relay (1.0)
logp	6.851		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2283.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	625.52	K	Cheméo Relay (1.0)
tf	259.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.66	J/mol×K	810.27	Joback Method
cpg	1042.54	J/mol×K	1004.22	Joback Method
cpg	1028.95	J/mol×K	971.89	Joback Method
cpg	1014.39	J/mol×K	939.57	Joback Method
cpg	998.82	J/mol×K	907.24	Joback Method
cpg	982.20	J/mol×K	874.92	Joback Method
cpg	964.50	J/mol×K	842.59	Joback Method
dvisc	0.0001476	Pa×s	622.03	Joback Method
dvisc	0.0000525	Pa×s	810.27	Joback Method

dvisc	0.0000699	Pa×s	747.52	Joback Method
dvisc	0.0000982	Pa×s	684.78	Joback Method
dvisc	0.0010196	Pa×s	433.80	Joback Method
dvisc	0.0002433	Pa×s	559.29	Joback Method
dvisc	0.0004550	Pa×s	496.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299796&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

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