o-Toluic acid, pentadecyl ester

Other names: o-Toluylic acid, pentadecyl ester
Inchi: InChI=1S/C23H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-17-20-25-23(24)22-19-16-15-18-2
InchiKey: WPBVGEFNCHWJHB-UHFFFAOYSA-N
Formula: C23H38O2
SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]: 346.55

Physical Properties

Property code	Value	Unit	Source
gf	11.64	kJ/mol	Joback Method
hf	-537.79	kJ/mol	Joback Method
hfus	51.76	kJ/mol	Joback Method
hvap	78.89	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.243		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2559.40		NIST Webbook
rinpol	2559.40		NIST Webbook
tb	833.59	K	Joback Method
tc	1027.34	K	Joback Method
tf	460.07	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.00	J/mol×K	833.59	Joback Method
cpg	1089.72	J/mol×K	995.05	Joback Method
cpg	1075.08	J/mol×K	962.76	Joback Method
cpg	1059.43	J/mol×K	930.47	Joback Method
cpg	1042.73	J/mol×K	898.17	Joback Method
cpg	1024.93	J/mol×K	865.88	Joback Method
cpg	1103.38	J/mol×K	1027.34	Joback Method

dvisc	0.0000498	Pa×s	833.59	Joback Method
dvisc	0.0000655	Pa×s	771.34	Joback Method
dvisc	0.0000904	Pa×s	709.08	Joback Method
dvisc	0.0001326	Pa×s	646.83	Joback Method
dvisc	0.0002112	Pa×s	584.58	Joback Method
dvisc	0.0003758	Pa×s	522.32	Joback Method
dvisc	0.0007816	Pa×s	460.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292384&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