o-Toluic acid, tetradecyl ester

Other names: o-Toluylic acid, tetradecyl ester
Inchi: InChI=1S/C22H36O2/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-24-22(23)21-18-15-14-17-20(2
InchiKey: SZJVQMWOMBMELE-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	3.22	kJ/mol	Joback Method
hf	-517.15	kJ/mol	Joback Method
hfus	49.17	kJ/mol	Joback Method
hvap	76.66	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.853		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1135.20	kPa	Joback Method
rinpol	2470.60		NIST Webbook
tb	810.71	K	Joback Method
tc	1003.02	K	Joback Method
tf	448.80	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.18	J/mol×K	810.71	Joback Method
cpg	1027.96	J/mol×K	970.97	Joback Method
cpg	1013.45	J/mol×K	938.92	Joback Method
cpg	997.95	J/mol×K	906.87	Joback Method
cpg	981.43	J/mol×K	874.81	Joback Method
cpg	963.86	J/mol×K	842.76	Joback Method
cpg	1041.52	J/mol×K	1003.02	Joback Method
dvisc	0.0000571	Pa×s	810.71	Joback Method

dvisc	0.0000749	Pa×s	750.39	Joback Method
dvisc	0.0001030	Pa×s	690.07	Joback Method
dvisc	0.0001505	Pa×s	629.75	Joback Method
dvisc	0.0002383	Pa×s	569.44	Joback Method
dvisc	0.0004208	Pa×s	509.12	Joback Method
dvisc	0.0008656	Pa×s	448.80	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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