m-Toluic acid, 2-tetradecyl ester

Other names: m-Toluylic acid, 2-tetradecyl ester
Inchi: InChI=1S/C22H36O2/c1-4-5-6-7-8-9-10-11-12-13-16-20(3)24-22(23)21-17-14-15-19(2)18
InchiKey: FGUNFUYYPHRHCT-UHFFFAOYSA-N
Formula: C22H36O2
SMILES: CCCCCCCCCCCCC(C)OC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	0.78	kJ/mol	Joback Method
hf	-522.43	kJ/mol	Joback Method
hfus	45.65	kJ/mol	Joback Method
hvap	76.27	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	6.851		Crippen Method
mcvol	304.520	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	810.27	K	Joback Method
tc	1004.22	K	Joback Method
tf	433.80	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0010196	Pa×s	433.80	Joback Method
dvisc	0.0004550	Pa×s	496.55	Joback Method
dvisc	0.0002433	Pa×s	559.29	Joback Method
dvisc	0.0001476	Pa×s	622.03	Joback Method
dvisc	0.0000982	Pa×s	684.78	Joback Method
dvisc	0.0000699	Pa×s	747.52	Joback Method
dvisc	0.0000525	Pa×s	810.27	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U299782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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