m-Toluic acid, 4-pentadecyl ester

Other names: m-Toluylic acid, 4-pentadecyl ester
Inchi: InChI=1S/C23H38O2/c1-4-6-7-8-9-10-11-12-13-18-22(15-5-2)25-23(24)21-17-14-16-20(3
InchiKey: LALIITKVHBOZJB-UHFFFAOYSA-N
Formula: C23H38O2
SMILES: CCCCCCCCCCCC(CCC)OC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 346.55

Physical Properties

Property code	Value	Unit	Source
gf	9.20	kJ/mol	Joback Method
hf	-543.07	kJ/mol	Joback Method
hfus	48.24	kJ/mol	Joback Method
hvap	78.50	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	7.241		Crippen Method
mcvol	318.610	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	833.15	K	Joback Method
tc	1028.23	K	Joback Method
tf	445.07	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.47	J/mol×K	833.15	Joback Method
cpg	1025.53	J/mol×K	865.66	Joback Method
cpg	1043.42	J/mol×K	898.18	Joback Method
cpg	1060.20	J/mol×K	930.69	Joback Method
cpg	1075.90	J/mol×K	963.20	Joback Method
cpg	1090.56	J/mol×K	995.71	Joback Method
cpg	1104.22	J/mol×K	1028.23	Joback Method
dvisc	0.0009154	Pa×s	445.07	Joback Method

dvisc	0.0004045	Pa×s	509.75	Joback Method
dvisc	0.0002149	Pa×s	574.43	Joback Method
dvisc	0.0001297	Pa×s	639.11	Joback Method
dvisc	0.0000859	Pa×s	703.79	Joback Method
dvisc	0.0000610	Pa×s	768.47	Joback Method
dvisc	0.0000457	Pa×s	833.15	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=U299788&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

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