

m-Toluic acid, pentadecyl ester

Other names:	m-Toluylic acid, pentadecyl ester
Inchi:	InChI=1S/C23H38O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-25-23(24)22-18-16-17-21(2)
InchiKey:	XKAKCFFKCDQFSB-UHFFFAOYSA-N
Formula:	C23H38O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1cccc(C)c1
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	2577.40		NIST Webbook
rinpol	2577.40		NIST Webbook
tb	833.59	K	Joback Method
tc	1027.34	K	Joback Method
tf	460.07	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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