

m-Toluylic acid, 4-tetradecyl ester

Inchi:	InChI=1S/C22H36O2/c1-4-6-7-8-9-10-11-12-17-21(14-5-2)24-22(23)20-16-13-15-19(3)18
InchiKey:	CQSDHNDMLCYZLD-UHFFFAOYSA-N
Formula:	C22H36O2
SMILES:	CCCCCCCCCCC(CCC)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	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	810.27	K	Joback Method
tc	1004.22	K	Joback Method
tf	433.80	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.66	J/molxK	810.27	Joback Method
cpg	964.50	J/molxK	842.59	Joback Method
cpg	982.20	J/molxK	874.92	Joback Method
cpg	998.82	J/molxK	907.24	Joback Method
cpg	1014.39	J/molxK	939.57	Joback Method
cpg	1028.95	J/molxK	971.89	Joback Method
cpg	1042.54	J/molxK	1004.22	Joback Method
dvisc	0.0010196	Paxs	433.80	Joback Method

dvisc	0.0004550	Paxs	496.55	Joback Method
dvisc	0.0002433	Paxs	559.29	Joback Method
dvisc	0.0001476	Paxs	622.03	Joback Method
dvisc	0.0000982	Paxs	684.78	Joback Method
dvisc	0.0000699	Paxs	747.52	Joback Method
dvisc	0.0000525	Paxs	810.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299784&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
mccvol:	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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