m-Toluic acid, tridecyl ester

Other names: m-Toluylic acid, tridecyl ester
Inchi: InChI=1S/C21H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-17-23-21(22)20-16-14-15-19(2)18-20
InchiKey: LNPAWBGTNBQFCH-UHFFFAOYSA-N
Formula: C21H34O2
SMILES: CCCCCCCCCCCCCOC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	-5.20	kJ/mol	Joback Method
hf	-496.51	kJ/mol	Joback Method
hfus	46.58	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	6.463		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2396.10		NIST Webbook
tb	787.83	K	Joback Method
tc	979.38	K	Joback Method
tf	437.53	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.17	J/mol×K	787.83	Joback Method
cpg	967.02	J/mol×K	947.45	Joback Method
cpg	952.64	J/mol×K	915.53	Joback Method
cpg	937.30	J/mol×K	883.60	Joback Method
cpg	920.96	J/mol×K	851.68	Joback Method
cpg	903.60	J/mol×K	819.75	Joback Method
cpg	980.48	J/mol×K	979.38	Joback Method
dvisc	0.0000654	Pa×s	787.83	Joback Method

dvisc	0.0000854	Pa×s	729.45	Joback Method
dvisc	0.0001170	Pa×s	671.06	Joback Method
dvisc	0.0001702	Pa×s	612.68	Joback Method
dvisc	0.0002679	Pa×s	554.30	Joback Method
dvisc	0.0004692	Pa×s	495.91	Joback Method
dvisc	0.0009543	Pa×s	437.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292359&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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