

p-Toluic acid, 3-tridecyl ester

Other names:	p-Toluylic acid, 3-tridecyl ester
Inchi:	InChI=1S/C21H34O2/c1-4-6-7-8-9-10-11-12-13-20(5-2)23-21(22)19-16-14-18(3)15-17-19
InchiKey:	NIWAOHOUTMSHPI-UHFFFAOYSA-N
Formula:	C21H34O2
SMILES:	CCCCCCCCCCC(CC)OC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	318.49

Physical Properties

Property code	Value	Unit	Source
gf	-7.64	kJ/mol	Joback Method
hf	-501.79	kJ/mol	Joback Method
hfus	43.06	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	6.461		Crippen Method
mcvol	290.430	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	787.39	K	Joback Method
tc	980.88	K	Joback Method
tf	422.53	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.66	J/molxK	787.39	Joback Method
cpg	904.28	J/molxK	819.64	Joback Method
cpg	921.80	J/molxK	851.89	Joback Method
cpg	938.27	J/molxK	884.13	Joback Method
cpg	953.71	J/molxK	916.38	Joback Method
cpg	968.16	J/molxK	948.63	Joback Method
cpg	981.66	J/molxK	980.88	Joback Method

dvisc	0.0011307	Paxs	422.53	Joback Method
dvisc	0.0005097	Paxs	483.34	Joback Method
dvisc	0.0002745	Paxs	544.15	Joback Method
dvisc	0.0001674	Paxs	604.96	Joback Method
dvisc	0.0001118	Paxs	665.77	Joback Method
dvisc	0.0000799	Paxs	726.58	Joback Method
dvisc	0.0000601	Paxs	787.39	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=U299803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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