

p-Toluic acid, hexyl ester

Other names:	Hexyl 4-methylbenzoate p-Toluylic acid, hexyl ester
Inchi:	InChI=1S/C14H20O2/c1-3-4-5-6-11-16-14(15)13-9-7-12(2)8-10-13/h7-10H,3-6,11H2,1-2
InchiKey:	PELWVATUYGIRES-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CCCCCCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	220.31
CAS:	27942-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-64.14	kJ/mol	Joback Method
hf	-352.03	kJ/mol	Joback Method
hfus	28.46	kJ/mol	Joback Method
hvap	58.85	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.732		Crippen Method
mvol	191.800	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1703.40		NIST Webbook
rinpol	1703.40		NIST Webbook
tb	627.67	K	Joback Method
tc	828.65	K	Joback Method
tf	358.64	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	493.85	J/molxK	627.67	Joback Method
cpg	509.98	J/molxK	661.17	Joback Method
cpg	525.23	J/molxK	694.66	Joback Method
cpg	539.64	J/molxK	728.16	Joback Method
cpg	553.21	J/molxK	761.65	Joback Method

cpg	565.96	J/molxK	795.15	Joback Method
cpg	577.93	J/molxK	828.65	Joback Method
dvisc	0.0015939	Paxs	358.64	Joback Method
dvisc	0.0008632	Paxs	403.48	Joback Method
dvisc	0.0005285	Paxs	448.32	Joback Method
dvisc	0.0003538	Paxs	493.16	Joback Method
dvisc	0.0002532	Paxs	537.99	Joback Method
dvisc	0.0001908	Paxs	582.83	Joback Method
dvisc	0.0001497	Paxs	627.67	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=C27942638&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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