

p-Toluic acid, heptyl ester

Other names:	p-Toluylic acid, heptyl ester
Inchi:	InChI=1S/C15H22O2/c1-3-4-5-6-7-12-17-15(16)14-10-8-13(2)9-11-14/h8-11H,3-7,12H2,
InchiKey:	XPCXKYHMNRJMRA-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCCCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	234.33
CAS:	331810-92-5

Physical Properties

Property code	Value	Unit	Source
gf	-55.72	kJ/mol	Joback Method
hf	-372.67	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.122		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1801.30		NIST Webbook
rinpol	1801.30		NIST Webbook
tb	650.55	K	Joback Method
tc	848.93	K	Joback Method
tf	369.91	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.11	J/molxK	650.55	Joback Method
cpg	562.71	J/molxK	683.61	Joback Method
cpg	578.41	J/molxK	716.68	Joback Method
cpg	593.23	J/molxK	749.74	Joback Method
cpg	607.19	J/molxK	782.80	Joback Method
cpg	620.31	J/molxK	815.87	Joback Method

cpg	632.62	J/mol×K	848.93	Joback Method
dvisc	0.0015149	Paxs	369.91	Joback Method
dvisc	0.0008075	Paxs	416.68	Joback Method
dvisc	0.0004887	Paxs	463.46	Joback Method
dvisc	0.0003243	Paxs	510.23	Joback Method
dvisc	0.0002306	Paxs	557.00	Joback Method
dvisc	0.0001728	Paxs	603.78	Joback Method
dvisc	0.0001350	Paxs	650.55	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=C331810925&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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