

p-Toluic acid, decyl ester

Other names:	p-Toluylic acid, decyl ester
Inchi:	InChI=1S/C18H28O2/c1-3-4-5-6-7-8-9-10-15-20-18(19)17-13-11-16(2)12-14-17/h11-14H
InchiKey:	QAISVFSPKQPVRM-UHFFFAOYSA-N
Formula:	C18H28O2
SMILES:	CCCCCCCCCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	276.41
CAS:	66606-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-30.46	kJ/mol	Joback Method
hf	-434.59	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.293		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2127.90		NIST Webbook
tb	719.19	K	Joback Method
tc	912.00	K	Joback Method
tf	403.72	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.68	J/molxK	719.19	Joback Method
cpg	728.33	J/molxK	751.33	Joback Method
cpg	745.01	J/molxK	783.46	Joback Method
cpg	760.73	J/molxK	815.60	Joback Method
cpg	775.53	J/molxK	847.73	Joback Method
cpg	789.43	J/molxK	879.87	Joback Method
cpg	802.46	J/molxK	912.00	Joback Method

dvisc	0.0012384	Paxs	403.72	Joback Method
dvisc	0.0006322	Paxs	456.30	Joback Method
dvisc	0.0003708	Paxs	508.88	Joback Method
dvisc	0.0002404	Paxs	561.46	Joback Method
dvisc	0.0001678	Paxs	614.03	Joback Method
dvisc	0.0001240	Paxs	666.61	Joback Method
dvisc	0.0000958	Paxs	719.19	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=C66606017&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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