

o-Toluic acid, undecyl ester

Other names:	o-toluylic acid, undecyl ester
Inchi:	InChI=1S/C19H30O2/c1-3-4-5-6-7-8-9-10-13-16-21-19(20)18-15-12-11-14-17(18)2/h11-17
InchiKey:	FORHRBUFDHOUGD-UHFFFAOYSA-N
Formula:	C19H30O2
SMILES:	CCCCCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	290.44

Physical Properties

Property code	Value	Unit	Source
gf	-22.04	kJ/mol	Joback Method
hf	-455.23	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.683		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2183.40		NIST Webbook
tb	742.07	K	Joback Method
tc	933.92	K	Joback Method
tf	414.99	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.84	J/molxK	742.07	Joback Method
cpg	847.73	J/molxK	901.95	Joback Method
cpg	833.64	J/molxK	869.97	Joback Method
cpg	818.64	J/molxK	838.00	Joback Method
cpg	802.70	J/molxK	806.02	Joback Method
cpg	785.77	J/molxK	774.05	Joback Method
cpg	860.92	J/molxK	933.92	Joback Method
dvisc	0.0000846	Paxs	742.07	Joback Method

dvisc	0.0001100	Paxs	687.56	Joback Method
dvisc	0.0001495	Paxs	633.04	Joback Method
dvisc	0.0002152	Paxs	578.53	Joback Method
dvisc	0.0003344	Paxs	524.02	Joback Method
dvisc	0.0005754	Paxs	469.50	Joback Method
dvisc	0.0011420	Paxs	414.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U292228&Units=SI

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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