

o-Toluic acid, 3,5-dimethylphenyl ester

Other names:	o-Toluylic acid, 3,5-dimethylphenyl ester
Inchi:	InChI=1S/C16H16O2/c1-11-8-12(2)10-14(9-11)18-16(17)15-7-5-4-6-13(15)3/h4-10H,1-3H
InchiKey:	KQHWCEXXLBPFGU-UHFFFAOYSA-N
Formula:	C16H16O2
SMILES:	<chem>Cc1cc(C)cc(OC(=O)c2ccccc2C)c1</chem>
Mol. weight [g/mol]:	240.30

Physical Properties

Property code	Value	Unit	Source
gf	45.85	kJ/mol	Joback Method
hf	-179.72	kJ/mol	Joback Method
hfus	26.90	kJ/mol	Joback Method
hvap	66.90	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.831		Crippen Method
mvol	196.220	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
rinpol	1911.00		NIST Webbook
rinpol	1911.00		NIST Webbook
tb	710.07	K	Joback Method
tc	945.48	K	Joback Method
tf	432.64	K	Joback Method
vc	0.740	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.08	J/mol×K	710.07	Joback Method
cpg	531.74	J/mol×K	749.31	Joback Method
cpg	546.25	J/mol×K	788.54	Joback Method
cpg	559.64	J/mol×K	827.78	Joback Method
cpg	571.96	J/mol×K	867.01	Joback Method
cpg	583.23	J/mol×K	906.25	Joback Method
cpg	593.49	J/mol×K	945.48	Joback Method

dvisc	0.0008112	Paxs	432.64	Joback Method
dvisc	0.0005079	Paxs	478.88	Joback Method
dvisc	0.0003453	Paxs	525.12	Joback Method
dvisc	0.0002499	Paxs	571.36	Joback Method
dvisc	0.0001898	Paxs	617.59	Joback Method
dvisc	0.0001498	Paxs	663.83	Joback Method
dvisc	0.0001219	Paxs	710.07	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=U307456&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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