1-Propanol, 3-(3,4,5-trimethoxyphenyl)

Inchi: InChI=1S/C12H18O4/c1-14-10-7-9(5-4-6-13)8-11(15-2)12(10)16-3/h7-8,13H,4-6H2,1-3H
InchiKey: IBRWTCISGCXHQZ-UHFFFAOYSA-N
Formula: C12H18O4
SMILES: COc1cc(CCCO)cc(OC)c1OC
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	-318.14	kJ/mol	Joback Method
hf	-637.78	kJ/mol	Joback Method
hfus	27.36	kJ/mol	Joback Method
hvap	70.48	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.637		Crippen Method
mcvol	179.660	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	675.02	K	Joback Method
tc	862.72	K	Joback Method
tf	416.49	K	Joback Method
vc	0.672	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.60	J/mol×K	675.02	Joback Method
cpg	495.47	J/mol×K	706.30	Joback Method
cpg	507.73	J/mol×K	737.59	Joback Method
cpg	519.38	J/mol×K	768.87	Joback Method
cpg	530.39	J/mol×K	800.15	Joback Method
cpg	540.76	J/mol×K	831.44	Joback Method
cpg	550.46	J/mol×K	862.72	Joback Method
dvisc	0.0006571	Pa×s	416.49	Joback Method

dvisc	0.0003052	Pa×s	459.58	Joback Method
dvisc	0.0001617	Pa×s	502.67	Joback Method
dvisc	0.0000947	Pa×s	545.75	Joback Method
dvisc	0.0000600	Pa×s	588.84	Joback Method
dvisc	0.0000404	Pa×s	631.93	Joback Method
dvisc	0.0000287	Pa×s	675.02	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=R220834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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