

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.60	J/molxK	675.02	Joback Method
cpg	540.76	J/molxK	831.44	Joback Method
cpg	530.39	J/molxK	800.15	Joback Method
cpg	519.38	J/molxK	768.87	Joback Method
cpg	507.73	J/molxK	737.59	Joback Method
cpg	495.47	J/molxK	706.30	Joback Method
cpg	550.46	J/molxK	862.72	Joback Method
dvisc	0.0000287	Paxs	675.02	Joback Method

dvisc	0.0000404	Paxs	631.93	Joback Method
dvisc	0.0000600	Paxs	588.84	Joback Method
dvisc	0.0000947	Paxs	545.75	Joback Method
dvisc	0.0001617	Paxs	502.67	Joback Method
dvisc	0.0003052	Paxs	459.58	Joback Method
dvisc	0.0006571	Paxs	416.49	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=R220834&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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