3-(3,4-DIMETHOXYPHENYL)-1-PROPANOL

Other names: Benzenepropanol, 3,4-dimethoxy-
1-Propanol, 3-(3,4-dimethoxyphenyl)
3-(3,4-dimethoxyphenyl)propanol
Inchi: InChI=1S/C11H16O3/c1-13-10-6-5-9(4-3-7-12)8-11(10)14-2/h5-6,8,12H,3-4,7H2,1-2H3
InchiKey: ZISWRXJZUKDIOO-UHFFFAOYSA-N
Formula: C11H16O3
SMILES: COc1ccc(CCCO)cc1OC
Mol. weight [g/mol]: 196.25

Physical Properties

Property code	Value	Unit	Source
hfus	23.97	kJ/mol	Joback Method
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-1.47		Cheméo Relay (1.0)
logp	1.629		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	593.76	K	Cheméo Relay (1.0)
tf	330.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.36	J/mol×K	624.74	Joback Method
cpg	419.81	J/mol×K	656.31	Joback Method
cpg	431.68	J/mol×K	687.88	Joback Method
cpg	442.97	J/mol×K	719.45	Joback Method
cpg	453.69	J/mol×K	751.02	Joback Method
cpg	463.83	J/mol×K	782.59	Joback Method
cpg	473.39	J/mol×K	814.16	Joback Method
dvisc	0.0016473	Pa×s	370.47	Joback Method
dvisc	0.0006711	Pa×s	412.85	Joback Method
dvisc	0.0003232	Pa×s	455.23	Joback Method

dvisc	0.0001762	Pa×s	497.61	Joback Method
dvisc	0.0001057	Pa×s	539.98	Joback Method
dvisc	0.0000683	Pa×s	582.36	Joback Method
dvisc	0.0000468	Pa×s	624.74	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3929473&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point