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]: 196.24
CAS: 3929-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-211.93	kJ/mol	Joback Method
hf	-473.45	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	1.629		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1661.00		NIST Webbook
tb	624.74	K	Joback Method
tc	814.16	K	Joback Method
tf	370.47	K	Joback Method
vc	0.599	m3/kmol	Joback Method

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

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=C3929473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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