

Benzenepropanol, 2-methoxy-

Other names:	1-Propanol, 3-(o-methoxyphenyl)- 3-o-Methoxyphenylpropan-1-ol 3-Guaiacyl propanol 3-(O-Methoxy phenyl)-1-propanol 2-Methoxyphenylpropanol
Inchi:	InChI=1S/C10H14O2/c1-12-10-7-3-2-5-9(10)6-4-8-11/h2-3,5,7,11H,4,6,8H2,1H3
InchiKey:	KCJSIKPCRQDRNX-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	COc1ccccc1CCCO
Mol. weight [g/mol]:	166.22
CAS:	10493-37-5

Physical Properties

Property code	Value	Unit	Source
gf	-105.72	kJ/mol	Joback Method
hf	-309.12	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.620		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1454.00		NIST Webbook
tb	574.46	K	Joback Method
tc	766.44	K	Joback Method
tf	324.45	K	Joback Method
vc	0.524	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.41	J/mol×K	574.46	Joback Method
cpg	389.74	J/mol×K	734.44	Joback Method
cpg	380.01	J/mol×K	702.45	Joback Method

cpg	369.72	J/molxK	670.45	Joback Method
cpg	358.87	J/molxK	638.45	Joback Method
cpg	347.43	J/molxK	606.46	Joback Method
cpg	398.94	J/molxK	766.44	Joback Method
dvisc	0.0000766	Paxs	574.46	Joback Method
dvisc	0.0001164	Paxs	532.79	Joback Method
dvisc	0.0001900	Paxs	491.12	Joback Method
dvisc	0.0003395	Paxs	449.46	Joback Method
dvisc	0.0006831	Paxs	407.79	Joback Method
dvisc	0.0016119	Paxs	366.12	Joback Method
dvisc	0.0047415	Paxs	324.45	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=C10493375&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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