Phenol, 2-methoxy-4-(methoxymethyl)-

Other names: Methyl vanillyl ether
2-methoxy-4-(methoxymethyl)phenol
Inchi: InChI=1S/C9H12O3/c1-11-6-7-3-4-8(10)9(5-7)12-2/h3-5,10H,6H2,1-2H3
InchiKey: USDDPDQEVLAOBO-UHFFFAOYSA-N
Formula: C9H12O3
SMILES: COCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 168.19
CAS: 5533-03-9

Physical Properties

Property code	Value	Unit	Source
gf	-236.94	kJ/mol	Joback Method
hf	-445.78	kJ/mol	Joback Method
hfus	20.88	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.547		Crippen Method
mcvol	131.520	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	562.44	K	Joback Method
tc	780.60	K	Joback Method
tf	386.31	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.71	J/mol×K	562.44	Joback Method
cpg	324.74	J/mol×K	598.80	Joback Method
cpg	336.12	J/mol×K	635.16	Joback Method
cpg	346.87	J/mol×K	671.52	Joback Method
cpg	357.03	J/mol×K	707.88	Joback Method
cpg	366.63	J/mol×K	744.24	Joback Method
cpg	375.72	J/mol×K	780.60	Joback Method

dvisc	0.0008400	Pa×s	386.31	Joback Method
dvisc	0.0004120	Pa×s	415.66	Joback Method
dvisc	0.0002220	Pa×s	445.02	Joback Method
dvisc	0.0001291	Pa×s	474.38	Joback Method
dvisc	0.0000800	Pa×s	503.73	Joback Method
dvisc	0.0000522	Pa×s	533.08	Joback Method
dvisc	0.0000357	Pa×s	562.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5533039&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume