O-Methoxy-«alpha»-methylbenzyl alcohol

Other names: 1-(O-Methoxyphenyl)ethanol
Benzenemethanol, 2-methoxy-«alpha»-methyl-
2-methoxy-alpha-methylbenzyl alcohol
Inchi: InChI=1S/C9H12O2/c1-7(10)8-5-3-4-6-9(8)11-2/h3-7,10H,1-2H3
InchiKey: DHHGVIOVURMJEA-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: COc1ccccc1C(C)O
Mol. weight [g/mol]: 152.19
CAS: 13513-82-1

Physical Properties

Property code	Value	Unit	Source
gf	-116.58	kJ/mol	Joback Method
hf	-293.76	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	57.27	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.748		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	551.14	K	Joback Method
tc	749.61	K	Joback Method
tf	298.18	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.88	J/mol×K	551.14	Joback Method
cpg	301.33	J/mol×K	584.22	Joback Method
cpg	312.20	J/mol×K	617.30	Joback Method
cpg	322.51	J/mol×K	650.37	Joback Method
cpg	332.27	J/mol×K	683.45	Joback Method
cpg	341.48	J/mol×K	716.53	Joback Method

cpg	350.17	J/mol×K	749.61	Joback Method
dvisc	0.0088416	Pa×s	298.18	Joback Method
dvisc	0.0025220	Pa×s	340.34	Joback Method
dvisc	0.0009485	Pa×s	382.50	Joback Method
dvisc	0.0004332	Pa×s	424.66	Joback Method
dvisc	0.0002279	Pa×s	466.82	Joback Method
dvisc	0.0001334	Pa×s	508.98	Joback Method
dvisc	0.0000847	Pa×s	551.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13513821&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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