3-Methoxybenzyl alcohol

Other names:	m-Methoxybenzyl alcohol
	Benzenemethanol, 3-methoxy-
Inchi:	InChI=1S/C8H10O2/c1-10-8-4-2-3-7(5-8)6-9/h2-5,9H,6H2,1H3
InchiKey:	IIGNZLVHOZEOPV-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	COc1cccc(CO)c1
Mol. weight [g/mol]:	138.16
CAS:	6971-51-3

Physical Properties

Property code	Value	Unit	Source
gf	-122.56	kJ/mol	Joback Method
hf	-267.84	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	55.43	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.188		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	1281.60		NIST Webbook
rinpol	1246.90		NIST Webbook
tb	528.70	K	Joback Method
tc	725.76	K	Joback Method
tf	301.91	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.43	J/mol×K	528.70	Joback Method
cpg	255.61	J/mol×K	561.54	Joback Method
cpg	265.29	J/mol×K	594.39	Joback Method
cpg	274.50	J/mol×K	627.23	Joback Method
cpg	283.23	J/mol×K	660.07	Joback Method

cpg	291.49	J/mol×K	692.92	Joback Method
cpg	299.29	J/mol×K	725.76	Joback Method
dvisc	0.0063822	Pa×s	301.91	Joback Method
dvisc	0.0022019	Pa×s	339.71	Joback Method
dvisc	0.0009401	Pa×s	377.51	Joback Method
dvisc	0.0004686	Pa×s	415.31	Joback Method
dvisc	0.0002624	Pa×s	453.10	Joback Method
dvisc	0.0001606	Pa×s	490.90	Joback Method
dvisc	0.0001055	Pa×s	528.70	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	523.20	K	96.40	NIST Webbook

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=C6971513&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume