

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/molxK	528.70	Joback Method
cpg	291.49	J/molxK	692.92	Joback Method
cpg	283.23	J/molxK	660.07	Joback Method
cpg	274.50	J/molxK	627.23	Joback Method
cpg	265.29	J/molxK	594.39	Joback Method

cpg	255.61	J/molxK	561.54	Joback Method
cpg	299.29	J/molxK	725.76	Joback Method
dvisc	0.0001055	Paxs	528.70	Joback Method
dvisc	0.0001606	Paxs	490.90	Joback Method
dvisc	0.0002624	Paxs	453.10	Joback Method
dvisc	0.0004686	Paxs	415.31	Joback Method
dvisc	0.0009401	Paxs	377.51	Joback Method
dvisc	0.0022019	Paxs	339.71	Joback Method
dvisc	0.0063822	Paxs	301.91	Joback Method

Pressure Dependent Properties

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

Sources

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=C6971513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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