3-Methylbenzyl alcohol

Other names:	m-Tolyl carbinol
	m-Methyl benzyl alcohol
	Benzenemethanol, 3-methyl-
Inchi:	InChI=1S/C8H10O/c1-7-3-2-4-8(5-7)6-9/h2-5,9H,6H2,1H3
InchiKey:	JJCKHVUTVOPLBV-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1cccc(CO)c1
Mol. weight [g/mol]:	122.16
CAS:	587-03-1

Physical Properties

Property code	Value	Unit	Source
gf	-17.56	kJ/mol	Joback Method
hf	-135.62	kJ/mol	Joback Method
hfus	14.22	kJ/mol	Joback Method
hvap	53.02	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.487		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1104.20		NIST Webbook
rinpol	1104.20		NIST Webbook
tb	506.28	K	Joback Method
tc	704.92	K	Joback Method
tf	279.68	K	Joback Method
vc	0.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.35	J/mol×K	506.28	Joback Method
cpg	233.69	J/mol×K	539.39	Joback Method
cpg	243.47	J/mol×K	572.49	Joback Method
cpg	252.73	J/mol×K	605.60	Joback Method

cpg	261.46	J/mol×K	638.71	Joback Method
cpg	269.71	J/mol×K	671.81	Joback Method
cpg	277.48	J/mol×K	704.92	Joback Method
dvisc	0.0114745	Pa×s	279.68	Joback Method
dvisc	0.0035387	Pa×s	317.45	Joback Method
dvisc	0.0014015	Pa×s	355.21	Joback Method
dvisc	0.0006632	Pa×s	392.98	Joback Method
dvisc	0.0003578	Pa×s	430.75	Joback Method
dvisc	0.0002133	Pa×s	468.51	Joback Method
dvisc	0.0001373	Pa×s	506.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	488.20	K	98.70	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=C587031&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