

3-METHYLBENZYL ALCOHOL

Other names:	3-methylbenzenemethanol Benzenemethanol, 3-methyl- m-Methyl benzyl alcohol m-Tolyl carbinol m-toluy alcohol
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]:	122.17

Physical Properties

Property code	Value	Unit	Source
af	0.5885		Cheméo Relay (1.0)
gf	-17.56	kJ/mol	Joback Method
hf	-144.16	kJ/mol	Cheméo Relay (1.0)
hfus	14.22	kJ/mol	Joback Method
hvap	71.80	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-1.05		Cheméo Relay (1.0)
logp	1.487		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1104.20		NIST Webbook
tb	474.74	K	Cheméo Relay (1.0)
tc	722.09	K	Cheméo Relay (1.0)
tf	264.30	K	Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry
vc	0.381	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.35	J/mol×K	506.28	Joback Method
cpg	277.48	J/mol×K	704.92	Joback Method
cpg	269.71	J/mol×K	671.81	Joback Method
cpg	261.46	J/mol×K	638.71	Joback Method
cpg	252.73	J/mol×K	605.60	Joback Method
cpg	243.47	J/mol×K	572.49	Joback Method
cpg	233.69	J/mol×K	539.39	Joback Method
dvisc	0.0006632	Pa×s	392.98	Joback Method
dvisc	0.0001373	Pa×s	506.28	Joback Method
dvisc	0.0002133	Pa×s	468.51	Joback Method
dvisc	0.0003578	Pa×s	430.75	Joback Method
dvisc	0.0114745	Pa×s	279.68	Joback Method
dvisc	0.0014015	Pa×s	355.21	Joback Method
dvisc	0.0035387	Pa×s	317.45	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Melting Point, Enthalpy of Fusion, and Heat Capacity Measurements of Several Polyfunctional, Industrially Important Compounds by Differential Scanning Calorimetry:

McGowan Method:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1021/acs.jced.7b01026>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C587031&Units=SI>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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