

Benzenemethanol, 4-methyl-

Other names:	1-(hydroxymethyl)-4-methylbenzene 4-(Hydroxymethyl)toluene 4-Methyl-1-hydroxymethylbenzene 4-Methyl-benzenemethanol 4-Methylbenzyl alcohol 4-Tolylcarbinol Benzyl alcohol, p-methyl- NSC 3992 p-Methylbenzyl alcohol p-Methylbenzylalkohol p-Toluy alcohol p-Tolylcarbinol
Inchi:	InChI=1S/C8H10O/c1-7-2-4-8(6-9)5-3-7/h2-5,9H,6H2,1H3
InchiKey:	KMTDMTZBANYGUNX-UHFFFAOYSA-N
Formula:	C8H10O
SMILES:	Cc1ccc(CO)cc1
Mol. weight [g/mol]:	122.16
CAS:	589-18-4

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	-1.20		Aqueous Solubility Prediction Method
logp	1.487		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1077.00		NIST Webbook
rinpol	1122.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1122.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1967.00		NIST Webbook

ripol	1977.00		NIST Webbook
ripol	1910.00		NIST Webbook
ripol	1960.00		NIST Webbook
tb	490.20	K	NIST Webbook
tc	719.00	K	Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method
tf	333.65	K	Aqueous Solubility Prediction Method
vc	0.395	m ³ /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	0.0035387	Paxs	317.45	Joback Method
dvisc	0.0114745	Paxs	279.68	Joback Method
dvisc	0.0014015	Paxs	355.21	Joback Method
dvisc	0.0006632	Paxs	392.98	Joback Method
dvisc	0.0003578	Paxs	430.75	Joback Method
dvisc	0.0002133	Paxs	468.51	Joback Method
dvisc	0.0001373	Paxs	506.28	Joback Method
hfust	20.17	kJ/mol	180.00	NIST Webbook
hvapt	64.20	kJ/mol	357.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C589184&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Vapor-liquid critical point measurements of fifteen compounds by the pulse-heating method: <https://www.doi.org/10.1016/j.fluid.2014.07.038>

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

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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