

3,4-DIMETHYLBENZYL ALCOHOL

Other names:	Benzenemethanol, 3,4-dimethyl-
Inchi:	InChI=1S/C9H12O/c1-7-3-4-9(6-10)5-8(7)2/h3-5,10H,6H2,1-2H3
InchiKey:	OKGZCXPDJKKZAP-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	Cc1ccc(CO)cc1C
Mol. weight [g/mol]:	136.19

Physical Properties

Property code	Value	Unit	Source
af	0.6248		Cheméo Relay (1.0)
gf	-18.77	kJ/mol	Joback Method
hf	-179.65	kJ/mol	Cheméo Relay (1.0)
hfus	16.42	kJ/mol	Joback Method
hvap	78.98	kJ/mol	Cheméo Relay (1.0)
ie	8.33	eV	Cheméo Relay (1.0)
log10ws	-1.71		Cheméo Relay (1.0)
logp	1.796		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1113.00		NIST Webbook
tb	492.70	K	NIST Webbook
tc	745.99	K	Cheméo Relay (1.0)
tf	305.37	K	Cheméo Relay (1.0)
vc	0.434	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.07	J/mol×K	534.14	Joback Method
cpg	324.37	J/mol×K	731.21	Joback Method
cpg	315.91	J/mol×K	698.37	Joback Method
cpg	306.97	J/mol×K	665.52	Joback Method
cpg	297.54	J/mol×K	632.68	Joback Method
cpg	287.59	J/mol×K	599.83	Joback Method

cpg	277.11	J/mol×K	566.99	Joback Method
dvisc	0.0004778	Pa×s	418.81	Joback Method
dvisc	0.0001123	Pa×s	534.14	Joback Method
dvisc	0.0001689	Pa×s	495.69	Joback Method
dvisc	0.0002719	Pa×s	457.25	Joback Method
dvisc	0.0061106	Pa×s	303.47	Joback Method
dvisc	0.0009411	Pa×s	380.36	Joback Method
dvisc	0.0021587	Pa×s	341.92	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6966105&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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