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
CAS: 6966-10-5

Physical Properties

Property code	Value	Unit	Source
gf	-18.77	kJ/mol	Joback Method
hf	-167.73	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.796		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
tb	492.70	K	NIST Webbook
tc	731.21	K	Joback Method
tf	303.47	K	Joback Method
vc	0.451	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.07	J/mol×K	534.14	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

cpg	324.37	J/mol×K	731.21	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	0.0004778	Pa×s	418.81	Joback Method
dvisc	0.0009411	Pa×s	380.36	Joback Method
dvisc	0.0021587	Pa×s	341.92	Joback Method
dvisc	0.0061106	Pa×s	303.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6966105&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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