3,5-Dimethylbenzylalcohol

Other names: Benzyl alcohol, 3,5-dimethyl-
3,5-Dimethylbenzyl alcohol
3,5-Dimethyl-1-hydroxymethylbenzene
3,5-Dimethylbenzenemethanol
Inchi: InChI=1S/C9H12O/c1-7-3-8(2)5-9(4-7)6-10/h3-5,10H,6H2,1-2H3
InchiKey: IQWWTJDRVBWBEL-UHFFFAOYSA-N
Formula: C9H12O
SMILES: Cc1cc(C)cc(CO)c1
Mol. weight [g/mol]: 136.19

Physical Properties

Property code	Value	Unit	Source
af	0.6307		Cheméo Relay (1.0)
gf	-18.77	kJ/mol	Joback Method
hf	-179.80	kJ/mol	Cheméo Relay (1.0)
hfus	16.42	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-1.66		Cheméo Relay (1.0)
logp	1.796		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	492.70	K	NIST Webbook
tc	733.46	K	Cheméo Relay (1.0)
tf	293.63	K	Cheméo Relay (1.0)
vc	0.437	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	277.11	J/mol×K	566.99	Joback Method
cpg	287.59	J/mol×K	599.83	Joback Method
cpg	297.54	J/mol×K	632.68	Joback Method

cpg	306.97	J/mol×K	665.52	Joback Method
cpg	315.91	J/mol×K	698.37	Joback Method
cpg	324.37	J/mol×K	731.21	Joback Method
dvisc	0.0061106	Pa×s	303.47	Joback Method
dvisc	0.0021587	Pa×s	341.92	Joback Method
dvisc	0.0009411	Pa×s	380.36	Joback Method
dvisc	0.0004778	Pa×s	418.81	Joback Method
dvisc	0.0002719	Pa×s	457.25	Joback Method
dvisc	0.0001689	Pa×s	495.69	Joback Method
dvisc	0.0001123	Pa×s	534.14	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27129879&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

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

Cheméo Relay (1.0):

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume