

2,5-DIMETHYLBENZYL ALCOHOL

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

Physical Properties

Property code	Value	Unit	Source
af	0.6147		Cheméo Relay (1.0)
gf	-18.77	kJ/mol	Joback Method
hf	-175.96	kJ/mol	Cheméo Relay (1.0)
hfus	16.42	kJ/mol	Joback Method
hvap	76.60	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-1.65		Cheméo Relay (1.0)
logp	1.796		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	506.20	K	NIST Webbook
tc	733.80	K	Cheméo Relay (1.0)
tf	321.00	K	Cheméo Relay (1.0)
vc	0.431	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53957338&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):	
Cheméo Relay (1.0, beta):	

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

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