3-HYDROXY-4-METHOXYBENZYL ALCOHOL

Other names: 4-Methoxy-3-hydroxy benzyl alcohol
Benzenemethanol, 3-hydroxy-4-methoxy-
Inchi: InChI=1S/C8H10O3/c1-11-8-3-2-6(5-9)4-7(8)10/h2-4,9-10H,5H2,1H3
InchiKey: WHKRHBLAJFYZKF-UHFFFAOYSA-N
Formula: C8H10O3
SMILES: COc1ccc(CO)cc1O
Mol. weight [g/mol]: 154.17

Physical Properties

Property code	Value	Unit	Source
hf	-418.80	kJ/mol	Cheméo Relay (1.0)
hfus	21.19	kJ/mol	Joback Method
hvap	98.15	kJ/mol	Cheméo Relay (1.0)
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-0.90		Cheméo Relay (1.0)
logp	0.893		Crippen Method
mcvol	117.430	ml/mol	McGowan Method
rinpol	1477.90		NIST Webbook
tb	546.88	K	Cheméo Relay (1.0)
tf	361.03	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.75	J/mol×K	609.32	Joback Method
cpg	337.55	J/mol×K	817.37	Joback Method
cpg	330.61	J/mol×K	782.70	Joback Method
cpg	323.31	J/mol×K	748.02	Joback Method
cpg	315.62	J/mol×K	713.35	Joback Method
cpg	307.49	J/mol×K	678.67	Joback Method
cpg	298.88	J/mol×K	644.00	Joback Method
dvisc	0.0000644	Pa×s	511.48	Joback Method
dvisc	0.0000118	Pa×s	609.32	Joback Method
dvisc	0.0000195	Pa×s	576.71	Joback Method

dvisc	0.0000342	Pa×s	544.09	Joback Method
dvisc	0.0007825	Pa×s	413.63	Joback Method
dvisc	0.0001322	Pa×s	478.86	Joback Method
dvisc	0.0003013	Pa×s	446.25	Joback Method

Sources

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4383066&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point