4-HYDROXY-2-METHYLBENZALDEHYDE

Other names: Benzaldehyde, 4-hydroxy-2-methyl-
Inchi: InChI=1S/C8H8O2/c1-6-4-8(10)3-2-7(6)5-9/h2-5,10H,1H3
InchiKey: JDWWIEFMFPWBST-UHFFFAOYSA-N
Formula: C8H8O2
SMILES: Cc1cc(O)ccc1C=O
Mol. weight [g/mol]: 136.15

Physical Properties

Property code	Value	Unit	Source
hf	-252.39	kJ/mol	Cheméo Relay (1.0)
hfus	18.20	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Cheméo Relay (1.0)
ie	8.73	eV	Cheméo Relay (1.0)
log10ws	-1.14		Cheméo Relay (1.0)
logp	1.513		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
tb	539.79	K	Cheméo Relay (1.0)
tc	798.35	K	Cheméo Relay (1.0)
tf	375.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.56	J/mol×K	543.38	Joback Method
cpg	248.41	J/mol×K	581.85	Joback Method
cpg	257.53	J/mol×K	620.31	Joback Method
cpg	265.98	J/mol×K	658.78	Joback Method
cpg	273.85	J/mol×K	697.24	Joback Method
cpg	281.20	J/mol×K	735.71	Joback Method
cpg	288.11	J/mol×K	774.17	Joback Method
dvisc	0.0017717	Pa×s	372.58	Joback Method
dvisc	0.0008670	Pa×s	401.05	Joback Method
dvisc	0.0004664	Pa×s	429.51	Joback Method

dvisc	0.0002710	Pa×s	457.98	Joback Method
dvisc	0.0001678	Pa×s	486.45	Joback Method
dvisc	0.0001096	Pa×s	514.91	Joback Method
dvisc	0.0000748	Pa×s	543.38	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41438180&Units=SI

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