2-Hydroxy-5-methylbenzaldehyde

Other names: Benzaldehyde, 2-hydroxy-5-methyl-
5-methylsalicylaldehyde
Inchi: InChI=1S/C8H8O2/c1-6-2-3-8(10)7(4-6)5-9/h2-5,10H,1H3
InchiKey: ILEIUTCVWLYZOM-UHFFFAOYSA-N
Formula: C8H8O2
SMILES: Cc1ccc(O)c(C=O)c1
Mol. weight [g/mol]: 136.15
CAS: 613-84-3

Physical Properties

Property code	Value	Unit	Source
gf	-134.88	kJ/mol	Joback Method
hf	-246.28	kJ/mol	Joback Method
hfus	18.20	kJ/mol	Joback Method
hvap	56.07	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	1.513		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	4775.98	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	1402.00		NIST Webbook
tb	543.38	K	Joback Method
tc	774.17	K	Joback Method
tf	372.58	K	Joback Method
vc	0.358	m3/kmol	Joback Method

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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C613843&Units=SI

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