

Methyl 2-hydroxy-6-methoxybenzoate

Inchi:	InChI=1S/C9H10O4/c1-12-7-5-3-4-6(10)8(7)9(11)13-2/h3-5,10H,1-2H3
InchiKey:	YRJIMTHQIPOSJR-UHFFFAOYSA-N
Formula:	C9H10O4
SMILES:	COC(=O)c1c(O)cccc1OC
Mol. weight [g/mol]:	182.17
CAS:	22833-69-8

Physical Properties

Property code	Value	Unit	Source
gf	-365.86	kJ/mol	Joback Method
hf	-558.36	kJ/mol	Joback Method
hfus	22.48	kJ/mol	Joback Method
hvap	63.15	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
rinpol	1444.10		NIST Webbook
rinpol	1403.00		NIST Webbook
ripol	2235.00		NIST Webbook
tb	616.31	K	Joback Method
tc	841.94	K	Joback Method
tf	436.24	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/molxK	616.31	Joback Method
cpg	336.25	J/molxK	653.92	Joback Method
cpg	346.47	J/molxK	691.52	Joback Method
cpg	356.09	J/molxK	729.13	Joback Method
cpg	365.12	J/molxK	766.73	Joback Method
cpg	373.62	J/molxK	804.34	Joback Method

cpg	381.62	J/molxK	841.94	Joback Method
dvisc	0.0004335	Paxs	436.24	Joback Method
dvisc	0.0002352	Paxs	466.25	Joback Method
dvisc	0.0001374	Paxs	496.26	Joback Method
dvisc	0.0000854	Paxs	526.27	Joback Method
dvisc	0.0000558	Paxs	556.29	Joback Method
dvisc	0.0000381	Paxs	586.30	Joback Method
dvisc	0.0000270	Paxs	616.31	Joback Method

Sources

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=C22833698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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