Methyl 6-hydroxy-o-anisate

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]: 182.18

Physical Properties

Property code	Value	Unit	Source
af	0.6915		Cheméo Relay (1.0)
hf	-613.63	kJ/mol	Cheméo Relay (1.0)
hfus	22.48	kJ/mol	Joback Method
hvap	77.02	kJ/mol	Cheméo Relay (1.0)
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-2.52		Cheméo Relay (1.0)
logp	1.187		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	542.13	K	Cheméo Relay (1.0)
tc	771.86	K	Cheméo Relay (1.0)
tf	318.63	K	Cheméo Relay (1.0)
vc	0.476	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.39	J/mol×K	616.31	Joback Method
cpg	381.62	J/mol×K	841.94	Joback Method
cpg	373.62	J/mol×K	804.34	Joback Method
cpg	365.12	J/mol×K	766.73	Joback Method
cpg	356.09	J/mol×K	729.13	Joback Method
cpg	346.47	J/mol×K	691.52	Joback Method
cpg	336.25	J/mol×K	653.92	Joback Method
dvisc	0.0000854	Pa×s	526.28	Joback Method
dvisc	0.0000270	Pa×s	616.31	Joback Method

dvisc	0.0000381	Pa×s	586.30	Joback Method
dvisc	0.0000558	Pa×s	556.29	Joback Method
dvisc	0.0004335	Pa×s	436.24	Joback Method
dvisc	0.0001374	Pa×s	496.26	Joback Method
dvisc	0.0002352	Pa×s	466.25	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C22833698&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):

Legend

af: Acentric Factor
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
vc: Critical Volume