Benzenepropanoic acid, 4-hydroxy-3-methoxy, methyl ester

Inchi: InChI=1S/C11H14O4/c1-14-10-7-8(3-5-9(10)12)4-6-11(13)15-2/h3,5,7,12H,4,6H2,1-2H3
InchiKey: PDTCYIZPTRRYOT-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COC(=O)CCc1ccc(O)c(OC)c1
Mol. weight [g/mol]: 210.23
CAS: 56024-44-3

Physical Properties

Property code	Value	Unit	Source
gf	-349.02	kJ/mol	Joback Method
hf	-599.64	kJ/mol	Joback Method
hfus	27.66	kJ/mol	Joback Method
hvap	67.60	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.506		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1683.80		NIST Webbook
rinpol	1644.00		NIST Webbook
tb	662.07	K	Joback Method
tc	879.72	K	Joback Method
tf	458.78	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.72	J/mol×K	662.07	Joback Method
cpg	434.18	J/mol×K	698.34	Joback Method
cpg	445.92	J/mol×K	734.62	Joback Method
cpg	456.99	J/mol×K	770.89	Joback Method
cpg	467.41	J/mol×K	807.17	Joback Method
cpg	477.24	J/mol×K	843.44	Joback Method
cpg	486.51	J/mol×K	879.72	Joback Method

dvisc	0.0003177	Pa×s	458.78	Joback Method
dvisc	0.0001660	Pa×s	492.66	Joback Method
dvisc	0.0000943	Pa×s	526.54	Joback Method
dvisc	0.0000573	Pa×s	560.42	Joback Method
dvisc	0.0000369	Pa×s	594.31	Joback Method
dvisc	0.0000249	Pa×s	628.19	Joback Method
dvisc	0.0000175	Pa×s	662.07	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=C56024443&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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