Propyl 2-hydroxy-4-methoxy-6-methylbenzoate

Inchi: InChI=1S/C12H16O4/c1-4-5-16-12(14)11-8(2)6-9(15-3)7-10(11)13/h6-7,13H,4-5H2,1-3H

InchiKey: LCPRSHPZBRBFJG-UHFFFAOYSA-N

Formula: C12H16O4

SMILES: CCCOC(=O)c1c(C)cc(OC)cc1O

Mol. weight [g/mol]: 224.25

Physical Properties

Property code	Value	Unit	Source
gf	-350.23	kJ/mol	Joback Method
hf	-631.75	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	70.49	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.276		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1713.10		NIST Webbook
tb	689.93	K	Joback Method
tc	904.92	K	Joback Method
tf	482.57	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.99	J/mol×K	689.93	Joback Method
cpg	483.97	J/mol×K	725.76	Joback Method
cpg	496.24	J/mol×K	761.59	Joback Method
cpg	507.83	J/mol×K	797.42	Joback Method
cpg	518.78	J/mol×K	833.25	Joback Method
cpg	529.12	J/mol×K	869.09	Joback Method
cpg	538.88	J/mol×K	904.92	Joback Method
dvisc	0.0002094	Pa×s	482.57	Joback Method
dvisc	0.0001142	Pa×s	517.13	Joback Method

dvisc	0.0000672	Pa×s	551.69	Joback Method
dvisc	0.0000421	Pa×s	586.25	Joback Method
dvisc	0.0000278	Pa×s	620.81	Joback Method
dvisc	0.0000192	Pa×s	655.37	Joback Method
dvisc	0.0000137	Pa×s	689.93	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=U412483&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