Ethyl 2-hydroxy-4-methoxy-6-propylbenzoate

Inchi: InChI=1S/C13H18O4/c1-4-6-9-7-10(16-3)8-11(14)12(9)13(15)17-5-2/h7-8,14H,4-6H2,1-3
InchiKey: ZTEGMSJYDACIAV-UHFFFAOYSA-N
Formula: C13H18O4
SMILES: CCCc1cc(OC)cc(O)c1C(=O)OCC
Mol. weight [g/mol]: 238.28
CAS: 53530-26-0

Physical Properties

Property code	Value	Unit	Source
gf	-341.81	kJ/mol	Joback Method
hf	-652.39	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	72.71	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.530		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1803.10		NIST Webbook
rinpol	1803.10		NIST Webbook
tb	712.81	K	Joback Method
tc	924.67	K	Joback Method
tf	493.84	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.84	J/mol×K	712.81	Joback Method
cpg	536.41	J/mol×K	748.12	Joback Method
cpg	549.23	J/mol×K	783.43	Joback Method
cpg	561.36	J/mol×K	818.74	Joback Method
cpg	572.81	J/mol×K	854.05	Joback Method
cpg	583.64	J/mol×K	889.36	Joback Method
cpg	593.86	J/mol×K	924.67	Joback Method

dvisc	0.0001794	Pa×s	493.84	Joback Method
dvisc	0.0000962	Pa×s	530.34	Joback Method
dvisc	0.0000559	Pa×s	566.83	Joback Method
dvisc	0.0000347	Pa×s	603.33	Joback Method
dvisc	0.0000228	Pa×s	639.82	Joback Method
dvisc	0.0000156	Pa×s	676.31	Joback Method
dvisc	0.0000111	Pa×s	712.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53530260&Units=SI
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

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