3-Methoxy-5-propylphenol

Inchi: InChI=1S/C10H14O2/c1-3-4-8-5-9(11)7-10(6-8)12-2/h5-7,11H,3-4H2,1-2H3
InchiKey: ILWXLUGUJRYVST-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CCCc1cc(O)cc(OC)c1
Mol. weight [g/mol]: 166.22
CAS: 55136-70-4

Physical Properties

Property code	Value	Unit	Source
gf	-123.52	kJ/mol	Joback Method
hf	-334.20	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	56.22	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.353		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	1504.30		NIST Webbook
rinpol	1504.30		NIST Webbook
tb	562.90	K	Joback Method
tc	779.84	K	Joback Method
tf	375.35	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.00	J/mol×K	562.90	Joback Method
cpg	348.17	J/mol×K	599.06	Joback Method
cpg	360.57	J/mol×K	635.21	Joback Method
cpg	372.26	J/mol×K	671.37	Joback Method
cpg	383.28	J/mol×K	707.52	Joback Method
cpg	393.69	J/mol×K	743.68	Joback Method
cpg	403.54	J/mol×K	779.84	Joback Method

dvisc	0.0012473	Pa×s	375.35	Joback Method
dvisc	0.0005647	Pa×s	406.61	Joback Method
dvisc	0.0002863	Pa×s	437.87	Joback Method
dvisc	0.0001589	Pa×s	469.12	Joback Method
dvisc	0.0000949	Pa×s	500.38	Joback Method
dvisc	0.0000602	Pa×s	531.64	Joback Method
dvisc	0.0000402	Pa×s	562.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55136704&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

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