4-(3-Hexyl)phenol

Inchi: InChI=1S/C12H18O/c1-3-5-10(4-2)11-6-8-12(13)9-7-11/h6-10,13H,3-5H2,1-2H3
InchiKey: AFXYCMIKKCWXCT-UHFFFAOYSA-N
Formula: C12H18O
SMILES: CCCC(CC)c1ccc(O)cc1
Mol. weight [g/mol]: 178.27
CAS: 6925-42-4

Physical Properties

Property code	Value	Unit	Source
gf	5.51	kJ/mol	Joback Method
hf	-237.07	kJ/mol	Joback Method
hfus	23.14	kJ/mol	Joback Method
hvap	57.21	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.686		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	580.82	K	Joback Method
tc	796.40	K	Joback Method
tf	348.14	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.71	J/mol×K	580.82	Joback Method
cpg	474.88	J/mol×K	760.47	Joback Method
cpg	462.71	J/mol×K	724.54	Joback Method
cpg	449.78	J/mol×K	688.61	Joback Method
cpg	436.03	J/mol×K	652.68	Joback Method
cpg	421.37	J/mol×K	616.75	Joback Method
cpg	486.39	J/mol×K	796.40	Joback Method
dvisc	0.0000359	Pa×s	580.82	Joback Method
dvisc	0.0000589	Pa×s	542.04	Joback Method

dvisc	0.0001043	Pa×s	503.26	Joback Method
dvisc	0.0002034	Pa×s	464.48	Joback Method
dvisc	0.0004478	Pa×s	425.70	Joback Method
dvisc	0.0011551	Pa×s	386.92	Joback Method
dvisc	0.0036794	Pa×s	348.14	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=C6925424&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume