

3-(3-Hexyl)phenol

Inchi:	InChI=1S/C12H18O/c1-3-6-10(4-2)11-7-5-8-12(13)9-11/h5,7-10,13H,3-4,6H2,1-2H3
InchiKey:	YTJIDRUNAKXIFI-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CCCC(CC)c1cccc(O)c1
Mol. weight [g/mol]:	178.27
CAS:	97218-44-5

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/molxK	580.82	Joback Method
cpg	421.37	J/molxK	616.75	Joback Method
cpg	436.03	J/molxK	652.68	Joback Method
cpg	449.78	J/molxK	688.61	Joback Method
cpg	462.71	J/molxK	724.54	Joback Method
cpg	474.88	J/molxK	760.47	Joback Method
cpg	486.39	J/molxK	796.40	Joback Method
dvisc	0.0036794	Paxs	348.14	Joback Method
dvisc	0.0011551	Paxs	386.92	Joback Method

dvisc	0.0004478	Paxs	425.70	Joback Method
dvisc	0.0002034	Paxs	464.48	Joback Method
dvisc	0.0001043	Paxs	503.26	Joback Method
dvisc	0.0000589	Paxs	542.04	Joback Method
dvisc	0.0000359	Paxs	580.82	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=C97218445&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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