

4-(3-Pentyl)phenol

Inchi:	InChI=1S/C11H16O/c1-3-9(4-2)10-5-7-11(12)8-6-10/h5-9,12H,3-4H2,1-2H3
InchiKey:	NXNCTLHHTLIVRD-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCC(CC)c1ccc(O)cc1
Mol. weight [g/mol]:	164.24
CAS:	29528-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-2.91	kJ/mol	Joback Method
hf	-216.43	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.296		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	557.94	K	Joback Method
tc	777.32	K	Joback Method
tf	336.87	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.97	J/molxK	557.94	Joback Method
cpg	423.84	J/molxK	740.76	Joback Method
cpg	412.32	J/molxK	704.20	Joback Method
cpg	400.05	J/molxK	667.63	Joback Method
cpg	386.96	J/molxK	631.07	Joback Method
cpg	372.96	J/molxK	594.50	Joback Method
cpg	434.70	J/molxK	777.32	Joback Method
dvisc	0.0000452	Paxs	557.94	Joback Method
dvisc	0.0000744	Paxs	521.10	Joback Method

dvisc	0.0001322	Paxs	484.25	Joback Method
dvisc	0.0002578	Paxs	447.41	Joback Method
dvisc	0.0005672	Paxs	410.56	Joback Method
dvisc	0.0014575	Paxs	373.72	Joback Method
dvisc	0.0046044	Paxs	336.87	Joback Method

Sources

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=C29528334&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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