

4-(3-Decyl)phenol

Inchi:	InChI=1S/C16H26O/c1-3-5-6-7-8-9-14(4-2)15-10-12-16(17)13-11-15/h10-14,17H,3-9H2,
InchiKey:	GUBSKPOSWSMECJ-UHFFFAOYSA-N
Formula:	C16H26O
SMILES:	CCCCCCCC(CC)c1ccc(O)cc1
Mol. weight [g/mol]:	234.38
CAS:	17408-60-5

Physical Properties

Property code	Value	Unit	Source
gf	39.19	kJ/mol	Joback Method
hf	-319.63	kJ/mol	Joback Method
hfus	33.50	kJ/mol	Joback Method
hvap	66.11	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	5.246		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
tb	672.34	K	Joback Method
tc	875.08	K	Joback Method
tf	393.22	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.62	J/molxK	672.34	Joback Method
cpg	629.14	J/molxK	706.13	Joback Method
cpg	645.69	J/molxK	739.92	Joback Method
cpg	661.35	J/molxK	773.71	Joback Method
cpg	676.21	J/molxK	807.50	Joback Method
cpg	690.33	J/molxK	841.29	Joback Method
cpg	703.80	J/molxK	875.08	Joback Method
dvisc	0.0015113	Paxs	393.22	Joback Method
dvisc	0.0004625	Paxs	439.74	Joback Method

dvisc	0.0001775	Paxs	486.26	Joback Method
dvisc	0.0000806	Paxs	532.78	Joback Method
dvisc	0.0000415	Paxs	579.30	Joback Method
dvisc	0.0000236	Paxs	625.82	Joback Method
dvisc	0.0000145	Paxs	672.34	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=C17408605&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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