

4(1,1-Dimethylhexyl)phenol

Inchi:	InChI=1S/C14H22O/c1-4-5-6-11-14(2,3)12-7-9-13(15)10-8-12/h7-10,15H,4-6,11H2,1-3H
InchiKey:	BTTSZRJAGSFTPE-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CCCCC(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	27.63	kJ/mol	Joback Method
hf	-281.82	kJ/mol	Joback Method
hfus	24.43	kJ/mol	Joback Method
hvap	60.75	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	4.250		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1602.30		NIST Webbook
rinpol	1615.50		NIST Webbook
rinpol	1608.20		NIST Webbook
tb	623.79	K	Joback Method
tc	840.06	K	Joback Method
tf	388.10	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.44	J/molxK	623.79	Joback Method
cpg	525.59	J/molxK	659.84	Joback Method
cpg	541.61	J/molxK	695.88	Joback Method
cpg	556.61	J/molxK	731.93	Joback Method
cpg	570.70	J/molxK	767.97	Joback Method
cpg	584.00	J/molxK	804.02	Joback Method
cpg	596.60	J/molxK	840.06	Joback Method

dvisc	0.0015972	Paxs	388.10	Joback Method
dvisc	0.0005613	Paxs	427.38	Joback Method
dvisc	0.0002353	Paxs	466.66	Joback Method
dvisc	0.0001128	Paxs	505.94	Joback Method
dvisc	0.0000602	Paxs	545.23	Joback Method
dvisc	0.0000349	Paxs	584.51	Joback Method
dvisc	0.0000217	Paxs	623.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R433253&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
mvol:	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

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