

4-(2,2,4-Trimethylpentyl) phenol

Inchi:	InChI=1S/C14H22O/c1-11(2)9-10-14(3,4)12-5-7-13(15)8-6-12/h5-8,11,15H,9-10H2,1-4H
InchiKey:	RNWSQHCPJBUHPH-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)CCC(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	206.32

Physical Properties

Property code	Value	Unit	Source
gf	25.19	kJ/mol	Joback Method
hf	-287.10	kJ/mol	Joback Method
hfus	20.90	kJ/mol	Joback Method
hvap	60.36	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.106		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1519.00		NIST Webbook
tb	623.35	K	Joback Method
tc	844.06	K	Joback Method
tf	373.10	K	Joback Method
vc	0.660	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.87	J/molxK	623.35	Joback Method
cpg	526.41	J/molxK	660.13	Joback Method
cpg	542.77	J/molxK	696.92	Joback Method
cpg	558.07	J/molxK	733.70	Joback Method
cpg	572.41	J/molxK	770.49	Joback Method
cpg	585.91	J/molxK	807.27	Joback Method
cpg	598.69	J/molxK	844.06	Joback Method
dvisc	0.0024425	Paxs	373.10	Joback Method
dvisc	0.0007356	Paxs	414.81	Joback Method

dvisc	0.0002758	Paxs	456.52	Joback Method
dvisc	0.0001219	Paxs	498.22	Joback Method
dvisc	0.0000611	Paxs	539.93	Joback Method
dvisc	0.0000338	Paxs	581.64	Joback Method
dvisc	0.0000203	Paxs	623.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R423157&Units=SI

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
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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