

(1,1,3,3-tetramethylbutyl)phenol

Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-14(4,5)11-7-6-8-12(15)9-11/h6-9,15H,10H2,1-5H3
InchiKey:	VHSOMXOOWFXZSD-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)CC(C)(C)c1ccccc(O)c1
Mol. weight [g/mol]:	206.32
CAS:	27193-28-8

Physical Properties

Property code	Value	Unit	Source
gf	30.47	kJ/mol	Joback Method
hf	-290.57	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	59.46	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	4.106		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
tb	620.56	K	Joback Method
tc	849.86	K	Joback Method
tf	390.52	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.49	J/mol×K	620.56	Joback Method
cpg	589.65	J/mol×K	811.64	Joback Method
cpg	576.11	J/mol×K	773.42	Joback Method
cpg	561.68	J/mol×K	735.21	Joback Method
cpg	546.21	J/mol×K	696.99	Joback Method
cpg	529.53	J/mol×K	658.78	Joback Method
cpg	602.44	J/mol×K	849.86	Joback Method
dvisc	0.0000194	Pa×s	620.56	Joback Method
dvisc	0.0000319	Pa×s	582.22	Joback Method

dvisc	0.0000560	Pa×s	543.88	Joback Method
dvisc	0.0001072	Pa×s	505.54	Joback Method
dvisc	0.0002283	Pa×s	467.20	Joback Method
dvisc	0.0005565	Pa×s	428.86	Joback Method
dvisc	0.0016156	Pa×s	390.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27193288&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
mcvol:	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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