

Phenol, 4-(2,2,3,3-tetramethylbutyl)-

Inchi:	InChI=1S/C14H22O/c1-13(2,3)14(4,5)10-11-6-8-12(15)9-7-11/h6-9,15H,10H2,1-5H3
InchiKey:	FBUPLQJWXXGMOF-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)C(C)(C)Cc1ccc(O)cc1
Mol. weight [g/mol]:	206.32
CAS:	54932-78-4

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	-3.85		Crippen Method
logp	4.007		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
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/molxK	620.56	Joback Method
cpg	529.53	J/molxK	658.78	Joback Method
cpg	546.21	J/molxK	696.99	Joback Method
cpg	561.68	J/molxK	735.21	Joback Method
cpg	576.11	J/molxK	773.42	Joback Method
cpg	589.65	J/molxK	811.64	Joback Method

cpg	602.44	J/molxK	849.86	Joback Method
dvisc	0.0016156	Paxs	390.52	Joback Method
dvisc	0.0005565	Paxs	428.86	Joback Method
dvisc	0.0002283	Paxs	467.20	Joback Method
dvisc	0.0001072	Paxs	505.54	Joback Method
dvisc	0.0000560	Paxs	543.88	Joback Method
dvisc	0.0000319	Paxs	582.22	Joback Method
dvisc	0.0000194	Paxs	620.56	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=C54932784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
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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