

Phenol, 2-(1,1,3,3-tetramethylbutyl)-

Other names:	Phenol, 2-(1,1,3,3-tetramethylbutyl)-
Inchi:	InChI=1S/C14H22O/c1-13(2,3)10-14(4,5)11-8-6-7-9-12(11)15/h6-9,15H,10H2,1-5H3
InchiKey:	XSXWOBXNYNULJG-UHFFFAOYSA-N
Formula:	C14H22O
SMILES:	CC(C)(C)CC(C)(C)c1ccccc1O
Mol. weight [g/mol]:	206.33

Physical Properties

Property code	Value	Unit	Source
hf	-274.04	kJ/mol	Cheméo Relay (1.0)
hfus	17.01	kJ/mol	Joback Method
hvap	73.80	kJ/mol	Cheméo Relay (1.0)
ie	8.18	eV	Cheméo Relay (1.0)
logp	4.106		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
tb	546.65	K	Cheméo Relay (1.0)
tf	342.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.49	J/mol×K	620.56	Joback Method
cpg	602.44	J/mol×K	849.86	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
dvisc	0.0001072	Pa×s	505.54	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	0.0016156	Pa×s	390.52	Joback Method
dvisc	0.0002283	Pa×s	467.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3884955&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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