

Phenol, 4-(1,1,2-trimethylhexyl)

Inchi:	InChI=1S/C15H24O/c1-5-6-7-12(2)15(3,4)13-8-10-14(16)11-9-13/h8-12,16H,5-7H2,1-4H
InchiKey:	AFKNSHUNGGHCGN-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CCCCC(C)C(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	33.61	kJ/mol	Joback Method
hf	-307.74	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.496		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	646.23	K	Joback Method
tc	863.09	K	Joback Method
tf	384.37	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.90	J/molxK	646.23	Joback Method
cpg	578.81	J/molxK	682.37	Joback Method
cpg	595.55	J/molxK	718.52	Joback Method
cpg	611.26	J/molxK	754.66	Joback Method
cpg	626.04	J/molxK	790.81	Joback Method
cpg	640.01	J/molxK	826.95	Joback Method

cpg	653.27	J/mol×K	863.09	Joback Method
dvisc	0.0019247	Paxs	384.37	Joback Method
dvisc	0.0005760	Paxs	428.01	Joback Method
dvisc	0.0002155	Paxs	471.66	Joback Method
dvisc	0.0000953	Paxs	515.30	Joback Method
dvisc	0.0000478	Paxs	558.94	Joback Method
dvisc	0.0000265	Paxs	602.59	Joback Method
dvisc	0.0000159	Paxs	646.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591923&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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