

Phenol, 4-(1,2,2,3,3-pentamethylbutyl)

Inchi:	InChI=1S/C15H24O/c1-11(15(5,6)14(2,3)4)12-7-9-13(16)10-8-12/h7-11,16H,1-6H3
InchiKey:	IVJSPATVAFWTOL-UHFFFAOYSA-N
Formula:	C15H24O
SMILES:	CC(c1ccc(O)cc1)C(C)(C)C(C)(C)C
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	36.45	kJ/mol	Joback Method
hf	-316.49	kJ/mol	Joback Method
hfus	16.08	kJ/mol	Joback Method
hvap	61.29	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinsol	1752.00		NIST Webbook
tb	643.00	K	Joback Method
tc	872.59	K	Joback Method
tf	386.79	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.77	J/molxK	643.00	Joback Method
cpg	582.53	J/molxK	681.26	Joback Method
cpg	599.92	J/molxK	719.53	Joback Method
cpg	616.10	J/molxK	757.79	Joback Method
cpg	631.22	J/molxK	796.06	Joback Method
cpg	645.45	J/molxK	834.32	Joback Method
cpg	658.94	J/molxK	872.59	Joback Method
dvisc	0.0019516	Paxs	386.79	Joback Method
dvisc	0.0005700	Paxs	429.49	Joback Method

dvisc	0.0002080	Paxs	472.19	Joback Method
dvisc	0.0000897	Paxs	514.89	Joback Method
dvisc	0.0000440	Paxs	557.60	Joback Method
dvisc	0.0000239	Paxs	600.30	Joback Method
dvisc	0.0000141	Paxs	643.00	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=R592431&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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