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

Inchi: InChI=1S/C15H24O/c1-11(14(2,3)4)15(5,6)12-7-9-13(16)10-8-12/h7-11,16H,1-6H3
InchiKey: FESTUJZLOUTDRN-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC(C(C)(C)C)C(C)(C)c1ccc(O)cc1
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	-3.94		Crippen Method
logp	4.352		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.77	J/mol×K	643.00	Joback Method
cpg	582.53	J/mol×K	681.26	Joback Method
cpg	599.92	J/mol×K	719.53	Joback Method
cpg	616.10	J/mol×K	757.79	Joback Method
cpg	631.22	J/mol×K	796.06	Joback Method
cpg	645.45	J/mol×K	834.32	Joback Method
cpg	658.94	J/mol×K	872.59	Joback Method
dvisc	0.0019516	Pa×s	386.79	Joback Method

dvisc	0.0005700	Pa×s	429.49	Joback Method
dvisc	0.0002080	Pa×s	472.19	Joback Method
dvisc	0.0000897	Pa×s	514.89	Joback Method
dvisc	0.0000440	Pa×s	557.60	Joback Method
dvisc	0.0000239	Pa×s	600.30	Joback Method
dvisc	0.0000141	Pa×s	643.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R592020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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