Phenol, 4-[1-ethyl-1-(1-methylethyl)butyl]

Inchi: InChI=1S/C15H24O/c1-5-11-15(6-2,12(3)4)13-7-9-14(16)10-8-13/h7-10,12,16H,5-6,11H2
InchiKey: LCYQASYKWOKSAB-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCC(CC)(c1ccc(O)cc1)C(C)C
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	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1776.00		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/mol×K	646.23	Joback Method
cpg	578.81	J/mol×K	682.37	Joback Method
cpg	595.55	J/mol×K	718.52	Joback Method
cpg	611.26	J/mol×K	754.66	Joback Method
cpg	626.04	J/mol×K	790.81	Joback Method
cpg	640.01	J/mol×K	826.95	Joback Method
cpg	653.27	J/mol×K	863.09	Joback Method

dvisc	0.0019247	Pa×s	384.37	Joback Method
dvisc	0.0005760	Pa×s	428.01	Joback Method
dvisc	0.0002155	Pa×s	471.66	Joback Method
dvisc	0.0000953	Pa×s	515.30	Joback Method
dvisc	0.0000478	Pa×s	558.94	Joback Method
dvisc	0.0000265	Pa×s	602.59	Joback Method
dvisc	0.0000159	Pa×s	646.23	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=R592268&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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