Phenol, 4-[1-ethyl-2-methyl-1-(1-methylethyl)propyl]

Inchi: InChI=1S/C15H24O/c1-6-15(11(2)3,12(4)5)13-7-9-14(16)10-8-13/h7-12,16H,6H2,1-5H3

InchiKey: POSPJEXWJFBONL-UHFFFAOYSA-N

Formula: C15H24O

SMILES: CCC(c1ccc(O)cc1)(C(C)C)C(C)C

Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	31.17	kJ/mol	Joback Method
hf	-313.02	kJ/mol	Joback Method
hfus	19.97	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	4.352		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2177.49	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	645.79	K	Joback Method
tc	866.98	K	Joback Method
tf	369.37	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.35	J/mol×K	645.79	Joback Method
cpg	579.65	J/mol×K	682.65	Joback Method
cpg	596.74	J/mol×K	719.52	Joback Method
cpg	612.74	J/mol×K	756.38	Joback Method
cpg	627.76	J/mol×K	793.25	Joback Method
cpg	641.94	J/mol×K	830.11	Joback Method
cpg	655.38	J/mol×K	866.98	Joback Method
dvisc	0.0030151	Pa×s	369.37	Joback Method

dvisc	0.0007611	Pa×s	415.44	Joback Method
dvisc	0.0002529	Pa×s	461.51	Joback Method
dvisc	0.0001026	Pa×s	507.58	Joback Method
dvisc	0.0000484	Pa×s	553.65	Joback Method
dvisc	0.0000256	Pa×s	599.72	Joback Method
dvisc	0.0000148	Pa×s	645.79	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=R592733&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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