Phenol, 4-(1-ethyl-1-propylbutyl)

Inchi: InChI=1S/C15H24O/c1-4-11-15(6-3,12-5-2)13-7-9-14(16)10-8-13/h7-10,16H,4-6,11-12H2
InchiKey: LAVCIELNPKVPFP-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCC(CC)(CCC)c1ccc(O)cc1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	36.05	kJ/mol	Joback Method
hf	-302.46	kJ/mol	Joback Method
hfus	27.02	kJ/mol	Joback Method
hvap	62.98	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.640		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1764.00		NIST Webbook
tb	646.67	K	Joback Method
tc	859.37	K	Joback Method
tf	399.37	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.46	J/mol×K	646.67	Joback Method
cpg	577.98	J/mol×K	682.12	Joback Method
cpg	594.40	J/mol×K	717.57	Joback Method
cpg	609.82	J/mol×K	753.02	Joback Method
cpg	624.36	J/mol×K	788.47	Joback Method
cpg	638.12	J/mol×K	823.92	Joback Method
cpg	651.21	J/mol×K	859.37	Joback Method
dvisc	0.0012837	Pa×s	399.37	Joback Method

dvisc	0.0004464	Pa×s	440.59	Joback Method
dvisc	0.0001860	Pa×s	481.80	Joback Method
dvisc	0.0000889	Pa×s	523.02	Joback Method
dvisc	0.0000474	Pa×s	564.24	Joback Method
dvisc	0.0000275	Pa×s	605.45	Joback Method
dvisc	0.0000171	Pa×s	646.67	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=R592322&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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