Phenol, 4-[1-(1-methylethyl)hexyl]

Inchi: InChI=1S/C15H24O/c1-4-5-6-7-15(12(2)3)13-8-10-14(16)11-9-13/h8-12,15-16H,4-7H2,1-
InchiKey: GCGLOVNVSBJCPI-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCCCC(c1ccc(O)cc1)C(C)C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	28.33	kJ/mol	Joback Method
hf	-304.27	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	63.50	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.712		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	649.02	K	Joback Method
tc	858.39	K	Joback Method
tf	366.95	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.51	J/mol×K	649.02	Joback Method
cpg	576.02	J/mol×K	683.91	Joback Method
cpg	592.50	J/mol×K	718.81	Joback Method
cpg	608.04	J/mol×K	753.70	Joback Method
cpg	622.73	J/mol×K	788.60	Joback Method
cpg	636.64	J/mol×K	823.49	Joback Method
cpg	649.87	J/mol×K	858.39	Joback Method
dvisc	0.0028979	Pa×s	366.95	Joback Method

dvisc	0.0007553	Pa×s	413.96	Joback Method
dvisc	0.0002590	Pa×s	460.97	Joback Method
dvisc	0.0001083	Pa×s	507.99	Joback Method
dvisc	0.0000525	Pa×s	555.00	Joback Method
dvisc	0.0000285	Pa×s	602.01	Joback Method
dvisc	0.0000169	Pa×s	649.02	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=R592411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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