

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:	CCCCC(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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007553	Paxs	413.96	Joback Method
dvisc	0.0002590	Paxs	460.97	Joback Method
dvisc	0.0001083	Paxs	507.99	Joback Method
dvisc	0.0000525	Paxs	555.00	Joback Method
dvisc	0.0000285	Paxs	602.01	Joback Method
dvisc	0.0000169	Paxs	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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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