Phenol, 4-(1-methyl-1-propylpentyl)

Inchi: InChI=1S/C15H24O/c1-4-6-12-15(3,11-5-2)13-7-9-14(16)10-8-13/h7-10,16H,4-6,11-12H2
InchiKey: RTLDGOFIOZOJIE-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CCCCC(C)(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	1732.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1744.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R591998&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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