

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

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

HFAYMOYWUDXVOB-UHFFFAOYSA-N

C15H24O

CCCC(C(C)C)C(C)c1ccc(O)cc1

220.35

Physical Properties

Property code	Value	Unit	Source
gf	25.89	kJ/mol	Joback Method
hf	-309.55	kJ/mol	Joback Method
hfus	23.86	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.568		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1744.00		NIST Webbook
tb	648.58	K	Joback Method
tc	861.97	K	Joback Method
tf	351.95	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.96	J/mol×K	648.58	Joback Method
cpg	576.84	J/mol×K	684.14	Joback Method
cpg	593.65	J/mol×K	719.71	Joback Method
cpg	609.47	J/mol×K	755.27	Joback Method
cpg	624.40	J/mol×K	790.84	Joback Method
cpg	638.52	J/mol×K	826.40	Joback Method
cpg	651.91	J/mol×K	861.97	Joback Method
dvisc	0.0046742	Pa×s	351.95	Joback Method
dvisc	0.0010084	Pa×s	401.39	Joback Method

dvisc	0.0003045	Pa×s	450.83	Joback Method
dvisc	0.0001165	Pa×s	500.26	Joback Method
dvisc	0.0000530	Pa×s	549.70	Joback Method
dvisc	0.0000275	Pa×s	599.14	Joback Method
dvisc	0.0000157	Pa×s	648.58	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=R592837&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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