Phenol, 4-(1,1,2,2,3-pentamethylhexyl)

Inchi: InChI=1S/C17H28O/c1-7-8-13(2)16(3,4)17(5,6)14-9-11-15(18)12-10-14/h9-13,18H,7-8H2
InchiKey: BSHAVJLLESPAAH-UHFFFAOYSA-N
Formula: C17H28O
SMILES: CCCC(C)C(C)(C)C(C)(C)c1ccc(O)cc1
Mol. weight [g/mol]: 248.40

Physical Properties

Property code	Value	Unit	Source
gf	53.29	kJ/mol	Joback Method
hf	-357.77	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	5.132		Crippen Method
mcvol	232.500	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	688.76	K	Joback Method
tc	910.06	K	Joback Method
tf	409.33	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.25	J/mol×K	688.76	Joback Method
cpg	690.44	J/mol×K	725.64	Joback Method
cpg	708.38	J/mol×K	762.53	Joback Method
cpg	725.20	J/mol×K	799.41	Joback Method
cpg	741.07	J/mol×K	836.29	Joback Method
cpg	756.12	J/mol×K	873.18	Joback Method
cpg	770.51	J/mol×K	910.06	Joback Method
dvisc	0.0011840	Pa×s	409.33	Joback Method

dvisc	0.0003420	Pa×s	455.90	Joback Method
dvisc	0.0001244	Pa×s	502.47	Joback Method
dvisc	0.0000537	Pa×s	549.04	Joback Method
dvisc	0.0000264	Pa×s	595.62	Joback Method
dvisc	0.0000144	Pa×s	642.19	Joback Method
dvisc	0.0000085	Pa×s	688.76	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R592406&Units=SI

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