Benzonitrile, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-

Other names: Benzonitrile, 3,5-di-tert-butyl-4-hydroxy-
3,5-Di-t-butyl-4-hydroxybenzonitrile
3,5-Ditert-butyl-4-hydroxybenzonitrile

Inchi: InChI=1S/C15H21NO/c1-14(2,3)11-7-10(9-16)8-12(13(11)17)15(4,5)6/h7-8,17H,1-6H3

InchiKey: AKXIIOLURNATOC-UHFFFAOYSA-N

Formula: C15H21NO

SMILES: CC(C)(C)c1cc(C#N)cc(C(C)(C)C)c1O

Mol. weight [g/mol]: 231.33

CAS: 1988-88-1

Physical Properties

Property code	Value	Unit	Source
gf	152.81	kJ/mol	Joback Method
hf	-169.27	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.859		Crippen Method
mcvol	205.700	ml/mol	McGowan Method
pc	2075.54	kPa	Joback Method
tb	755.48	K	Joback Method
tc	993.41	K	Joback Method
tf	491.82	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.89	J/mol×K	755.48	Joback Method
cpg	605.44	J/mol×K	795.13	Joback Method
cpg	619.13	J/mol×K	834.79	Joback Method
cpg	632.13	J/mol×K	874.44	Joback Method
cpg	644.58	J/mol×K	914.10	Joback Method
cpg	656.64	J/mol×K	953.75	Joback Method

cpg	668.47	J/mol×K	993.41	Joback Method

Sources

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=C1988881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume