3,5-DI-t-BUTYL-4-HYDROXYBENZONITRILE

Other names: 3,5-Di-t-butyl-4-hydroxybenzonitrile
3,5-Ditert-butyl-4-hydroxybenzonitrile
Benzonitrile, 3,5-di-tert-butyl-4-hydroxy-
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]: 231.34

Physical Properties

Property code	Value	Unit	Source
hf	-150.46	kJ/mol	Cheméo Relay (1.0)
hfus	20.33	kJ/mol	Joback Method
hvap	87.42	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-4.78		Cheméo Relay (1.0)
logp	3.859		Crippen Method
mcvol	205.700	ml/mol	McGowan Method
tb	562.77	K	Cheméo Relay (1.0)
tf	418.16	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1988881&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point