Benzaldehyde, 2-hydroxy, 5-(1,1,3,3-tetramethylbutyl)

Inchi: InChI=1S/C15H22O2/c1-14(2,3)10-15(4,5)12-6-7-13(17)11(8-12)9-16/h6-9,17H,10H2,1-5

InchiKey: PRQGLXVKXBBFHU-UHFFFAOYSA-N

Formula: C15H22O2

SMILES: CC(C)(C)CC(C)(C)c1ccc(O)c(C=O)c1

Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	-70.26	kJ/mol	Joback Method
hf	-408.26	kJ/mol	Joback Method
hfus	21.50	kJ/mol	Joback Method
hvap	69.06	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.919		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1879.00		NIST Webbook
tb	697.08	K	Joback Method
tc	924.32	K	Joback Method
tf	456.31	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.43	J/mol×K	697.08	Joback Method
cpg	598.34	J/mol×K	734.95	Joback Method
cpg	613.17	J/mol×K	772.83	Joback Method
cpg	627.08	J/mol×K	810.70	Joback Method
cpg	640.21	J/mol×K	848.57	Joback Method
cpg	652.70	J/mol×K	886.44	Joback Method
cpg	664.69	J/mol×K	924.32	Joback Method
dvisc	0.0004992	Pa×s	456.31	Joback Method
dvisc	0.0002099	Pa×s	496.44	Joback Method

dvisc	0.0001004	Pa×s	536.57	Joback Method
dvisc	0.0000533	Pa×s	576.70	Joback Method
dvisc	0.0000307	Pa×s	616.82	Joback Method
dvisc	0.0000189	Pa×s	656.95	Joback Method
dvisc	0.0000123	Pa×s	697.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R256843&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

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

Latest version available from:
https://www.chemeo.com/cid/64-905-6/Benzaldehyde-2-hydroxy-5-1-1-3-3-tetramethylbutyl.pdf
Generated by Cheméo on 2024-10-12 06:56:42.260957449 +0000 UTC m=+3297064.897926707.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.