

Benzaldehyde, 2-hydroxy, 5-dodecyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-17-13-14-19(21)18(15-17)16-20/h13-1

GGHYSWAOXYBGNK-UHFFFAOYSA-N

C19H30O2

CCCCCCCCCCCCc1ccc(O)c(C=O)c1

290.44

Physical Properties

Property code	Value	Unit	Source
gf	-42.26	kJ/mol	Joback Method
hf	-473.32	kJ/mol	Joback Method
hfus	46.69	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.668		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2495.00		NIST Webbook
rinpol	2495.00		NIST Webbook
tb	795.06	K	Joback Method
tc	994.30	K	Joback Method
tf	496.55	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.07	J/mol×K	795.06	Joback Method
cpg	816.63	J/mol×K	828.27	Joback Method
cpg	832.39	J/mol×K	861.47	Joback Method
cpg	847.42	J/mol×K	894.68	Joback Method
cpg	861.81	J/mol×K	927.89	Joback Method
cpg	875.63	J/mol×K	961.09	Joback Method
cpg	888.95	J/mol×K	994.30	Joback Method
dvisc	0.0002760	Pa×s	496.55	Joback Method

dvisc	0.0001147	Pa×s	546.30	Joback Method
dvisc	0.0000552	Pa×s	596.05	Joback Method
dvisc	0.0000297	Pa×s	645.80	Joback Method
dvisc	0.0000175	Pa×s	695.56	Joback Method
dvisc	0.0000111	Pa×s	745.31	Joback Method
dvisc	0.0000074	Pa×s	795.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R256863&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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