DODECYL P-HYDROXYBENZOATE

Other names: n-Dodecyl 4-hydroxybenzoate
Benzoic acid, 4-hydroxy-, dodecyl ester
Benzoic acid, p-hydroxy-, dodecyl ester
Dodecyl 4-hydroxybenzoate
p-Hydroxybenzoic acid dodecyl ester
p-Oxybenzoesaureduodecylester

Inchi: InChI=1S/C19H30O3/c1-2-3-4-5-6-7-8-9-10-11-16-22-19(21)17-12-14-18(20)15-13-17/h1

InchiKey: BAYSQTBAJQRACX-UHFFFAOYSA-N

Formula: C19H30O3

SMILES: CCCCCCCCCCCCOC(=O)c1ccc(O)cc1

Mol. weight [g/mol]: 306.45

Physical Properties

Property code	Value	Unit	Source
af	1.0407		Cheméo Relay (1.0)
hf	-681.50	kJ/mol	Cheméo Relay (1.0)
hfus	47.58	kJ/mol	Joback Method
hvap	112.71	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-5.89		Cheméo Relay (1.0)
logp	5.470		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	636.87	K	Cheméo Relay (1.0)
tc	850.67	K	Cheméo Relay (1.0)
tf	353.19	K	Cheméo Relay (1.0)
vc	1.001	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.62	J/mol×K	817.71	Joback Method
cpg	847.12	J/mol×K	851.29	Joback Method
cpg	862.78	J/mol×K	884.86	Joback Method

cpg	877.65	J/mol×K	918.44	Joback Method
cpg	891.82	J/mol×K	952.01	Joback Method
cpg	905.34	J/mol×K	985.59	Joback Method
cpg	918.30	J/mol×K	1019.16	Joback Method
dvisc	0.0001720	Pa×s	514.19	Joback Method
dvisc	0.0000718	Pa×s	564.78	Joback Method
dvisc	0.0000346	Pa×s	615.36	Joback Method
dvisc	0.0000186	Pa×s	665.95	Joback Method
dvisc	0.0000110	Pa×s	716.54	Joback Method
dvisc	0.0000069	Pa×s	767.12	Joback Method
dvisc	0.0000046	Pa×s	817.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2664600&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

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume

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