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]:	306.44
CAS:	2664-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-167.03	kJ/mol	Joback Method
hf	-621.07	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	82.33	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	5.470		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1579.71	kPa	Joback Method
tb	817.71	K	Joback Method
tc	1019.16	K	Joback Method
tf	514.19	K	Joback Method
vc	0.982	m3/kmol	Joback Method

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

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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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