

Benzoic acid, 4-(dodecyloxy)-

Other names:	Benzoic acid, p-(dodecyloxy)- p-(Dodecyloxy)benzoic acid para-Dodecyloxybenzoic acid 4-n-Dodecyloxybenzoic acid 4-(dodecyloxy)benzoic acid
Inchi:	InChI=1S/C19H30O3/c1-2-3-4-5-6-7-8-9-10-11-16-22-18-14-12-17(13-15-18)19(20)21/h1
InchiKey:	ALQLYJHDBAKLBB-UHFFFAOYSA-N
Formula:	C19H30O3
SMILES:	CCCCCCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	306.44
CAS:	2312-15-4

Physical Properties

Property code	Value	Unit	Source
gf	-158.86	kJ/mol	Joback Method
hf	-607.46	kJ/mol	Joback Method
hfus	45.49	kJ/mol	Joback Method
hvap	86.66	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.684		Crippen Method
mcvol	268.120	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
tb	834.25	K	Joback Method
tc	1027.56	K	Joback Method
tf	475.81	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	835.00	J/mol×K	834.25	Joback Method
cpg	850.33	J/mol×K	866.47	Joback Method
cpg	864.72	J/mol×K	898.69	Joback Method
cpg	878.20	J/mol×K	930.90	Joback Method

cpg	890.80	J/mol×K	963.12	Joback Method
cpg	902.55	J/mol×K	995.34	Joback Method
cpg	913.49	J/mol×K	1027.56	Joback Method
dvisc	0.0006119	Pa×s	475.81	Joback Method
dvisc	0.0002302	Pa×s	535.55	Joback Method
dvisc	0.0001054	Pa×s	595.29	Joback Method
dvisc	0.0000556	Pa×s	655.03	Joback Method
dvisc	0.0000327	Pa×s	714.77	Joback Method
dvisc	0.0000208	Pa×s	774.51	Joback Method
dvisc	0.0000142	Pa×s	834.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2312154&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

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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