Acetic acid, 4-benzoyl-3-hydroxyphenoxy-, dodecyl ester

Inchi: InChI=1S/C27H36O5/c1-2-3-4-5-6-7-8-9-10-14-19-31-26(29)21-32-23-17-18-24(25(28)20
InchiKey: UHPRCGHAUHEORR-UHFFFAOYSA-N
Formula: C27H36O5
SMILES: CCCCCCCCCCCCOC(=O)COc1ccc(C(=O)c2ccccc2)c(O)c1
Mol. weight [g/mol]: 440.57
CAS: 103100-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-230.81	kJ/mol	Joback Method
hf	-805.93	kJ/mol	Joback Method
hfus	64.74	kJ/mol	Joback Method
hvap	112.24	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.466		Crippen Method
mcvol	364.520	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
tb	1108.70	K	Joback Method
tc	1357.72	K	Joback Method
tf	715.45	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.73	J/mol×K	1108.70	Joback Method
cpg	1329.08	J/mol×K	1316.22	Joback Method
cpg	1315.81	J/mol×K	1274.72	Joback Method
cpg	1302.08	J/mol×K	1233.21	Joback Method
cpg	1287.76	J/mol×K	1191.71	Joback Method
cpg	1272.69	J/mol×K	1150.20	Joback Method
cpg	1342.05	J/mol×K	1357.72	Joback Method
dvisc	0.0000005	Pa×s	1108.70	Joback Method
dvisc	0.0000007	Pa×s	1043.16	Joback Method

dvisc	0.0000011	Pa×s	977.62	Joback Method
dvisc	0.0000017	Pa×s	912.07	Joback Method
dvisc	0.0000029	Pa×s	846.53	Joback Method
dvisc	0.0000053	Pa×s	780.99	Joback Method
dvisc	0.0000109	Pa×s	715.45	Joback Method

Sources

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=C103100750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

https://www.chemeo.com/cid/92-142-2/Acetic-acid-4-benzoyl-3-hydroxyphenoxy-dodecyl-ester.pdf

Generated by Cheméo on 2024-10-12 07:23:03.717071439 +0000 UTC m=+3298646.354040687.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.