

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/molxK	1108.70	Joback Method
cpg	1329.08	J/molxK	1316.22	Joback Method
cpg	1315.81	J/molxK	1274.72	Joback Method
cpg	1302.08	J/molxK	1233.21	Joback Method
cpg	1287.76	J/molxK	1191.71	Joback Method
cpg	1272.69	J/molxK	1150.20	Joback Method
cpg	1342.05	J/molxK	1357.72	Joback Method
dvisc	0.0000005	Paxs	1108.70	Joback Method
dvisc	0.0000007	Paxs	1043.16	Joback Method

dvisc	0.0000011	Paxs	977.62	Joback Method
dvisc	0.0000017	Paxs	912.07	Joback Method
dvisc	0.0000029	Paxs	846.53	Joback Method
dvisc	0.0000053	Paxs	780.99	Joback Method
dvisc	0.0000109	Paxs	715.45	Joback Method

Sources

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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