

Benzophenone, 2-hydroxy-4-octadecyloxy-

Other names:	2-hydroxy-4-(octadecyloxy)benzophenone
Inchi:	InChI=1S/C31H46O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-25-34-28-23-24-29(30)
InchiKey:	POLSVAXEEHDBMJ-UHFFFAOYSA-N
Formula:	C31H46O3
SMILES:	CCCCCCCCCCCCCCCCCOc1ccc(C(=O)c2ccccc2)c(O)c1
Mol. weight [g/mol]:	466.70
CAS:	3457-13-4

Physical Properties

Property code	Value	Unit	Source
gf	36.79	kJ/mol	Joback Method
hf	-643.69	kJ/mol	Joback Method
hfus	72.31	kJ/mol	Joback Method
hvap	111.98	kJ/mol	Joback Method
log10ws	-10.21		Crippen Method
logp	9.264		Crippen Method
mcvol	413.440	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
tb	1123.93	K	Joback Method
tc	1381.03	K	Joback Method
tf	688.37	K	Joback Method
vc	1.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.31	J/molxK	1123.93	Joback Method
cpg	1575.15	J/molxK	1338.18	Joback Method
cpg	1555.79	J/molxK	1295.33	Joback Method
cpg	1536.33	J/molxK	1252.48	Joback Method
cpg	1516.58	J/molxK	1209.63	Joback Method
cpg	1496.31	J/molxK	1166.78	Joback Method
cpg	1594.64	J/molxK	1381.03	Joback Method
dvisc	0.0000004	Paxs	1123.93	Joback Method

dvisc	0.0000006	Paxs	1051.34	Joback Method
dvisc	0.0000009	Paxs	978.74	Joback Method
dvisc	0.0000015	Paxs	906.15	Joback Method
dvisc	0.0000027	Paxs	833.56	Joback Method
dvisc	0.0000054	Paxs	760.96	Joback Method
dvisc	0.0000127	Paxs	688.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3457134&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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