Oxybenzone

Other names:	Methanone, (2-hydroxy-4-methoxyphenyl)phenyl-
	Benzophenone, 2-hydroxy-4-methoxy-
	Advastab 45
	Anuvex
	Benzophenone-3
	Chimassorb 90
	Cyasorb uv 9
	Cyasorb uv 9 light absorber
	Mob
	Oxybenzon
	Spectra-sorb UV 9
	Sunscreen UV-15
	Uvinul M 40
	Uvinul 9
	Uvistat 24
	UF 3
	UV 9
	2-Hydroxy-4-methoxybenzophenone
	4-Methoxy-2-hydroxybenzophenone
	MOD
	Syntase 62
	USAF cy-9
	(2-Hydroxy-4-methoxyphenyl)phenylmethanone
	NCI-C60957
	NSC-7778
	2-Benzoyl-5-methoxyphenol
	Escalol 567
	Eusolex 4360
	HMBP
	Neo heliopan BB
	Ongrostab HMB
Inchi:	InChI=1S/C14H12O3/c1-17-11-7-8-12(13(15)9-11)14(16)10-5-3-2-4-6-10/h2-9,15H,1H3
InchiKey:	DXGLGDHPHMLXJC-UHFFFAOYSA-N
Formula:	C14H12O3
SMILES:	COc1ccc(C(=O)c2ccccc2)c(O)c1
Mol. weight [g/mol]:	228.24
CAS:	131-57-7

Physical Properties

Property code	Value	Unit	Source
gf	-106.35	kJ/mol	Joback Method
hf	-292.81	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	74.14	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.632		Crippen Method
mcvol	173.910	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	734.97	K	Joback Method
tc	985.71	K	Joback Method
tf	496.78	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.15	J/mol×K	943.92	Joback Method
cpg	498.98	J/mol×K	860.34	Joback Method
cpg	487.84	J/mol×K	818.55	Joback Method
cpg	475.85	J/mol×K	776.76	Joback Method
cpg	462.89	J/mol×K	734.97	Joback Method
cpg	509.38	J/mol×K	902.13	Joback Method
cpg	528.39	J/mol×K	985.71	Joback Method
dvisc	0.0002250	Pa×s	496.78	Joback Method
dvisc	0.0000118	Pa×s	734.97	Joback Method
dvisc	0.0000167	Pa×s	695.27	Joback Method
dvisc	0.0000248	Pa×s	655.57	Joback Method
dvisc	0.0000387	Pa×s	615.88	Joback Method
dvisc	0.0000641	Pa×s	576.18	Joback Method
dvisc	0.0001147	Pa×s	536.48	Joback Method
hfust	21.77	kJ/mol	336.70	NIST Webbook
hsubt	118.90	kJ/mol	309.00	NIST Webbook
hvapt	74.70	kJ/mol	375.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	0.70	NIST Webbook

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=C131577&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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume