Dioxybenzone

Other names:	Methanone, (2-hydroxy-4-methoxyphenyl)(2-hydroxyphenyl)-
	Benzophenone, 2,2'-dihydroxy-4-methoxy-
	Advastab 47
	Cyasorb UV 24
	Cyasorb UV 24 Light Absorber
	Dioxybenzon
	Spectra-Sorb UV 24
	UF 2
	UV 24
	2,2'-Dihydroxy-4-Methoxybenzophenone
	Benzophenone-8
	(2-Hydroxy-4-methoxyphenyl)(2-hydroxyphenyl)methanone
	NSC-56769
	Spectro-Sorb UV 24
Inchi:	InChI=1S/C14H12O4/c1-18-9-6-7-11(13(16)8-9)14(17)10-4-2-3-5-12(10)15/h2-8,15-16H,
InchiKey:	MEZZCSHVIGVWFI-UHFFFAOYSA-N
Formula:	C14H12O4
SMILES:	COc1ccc(C(=O)c2ccccc2O)c(O)c1
Mol. weight [g/mol]:	244.24
CAS:	131-53-3

Physical Properties

Property code	Value	Unit	Source
gf	-260.97	kJ/mol	Joback Method
hf	-470.12	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	87.16	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.337		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	4051.80	kPa	Joback Method
tb	815.59	K	Joback Method
tc	1072.05	K	Joback Method
tf	608.50	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.35	J/mol×K	1029.30	Joback Method
cpg	528.74	J/mol×K	901.08	Joback Method
cpg	517.54	J/mol×K	858.33	Joback Method
cpg	505.87	J/mol×K	815.59	Joback Method
cpg	539.66	J/mol×K	943.82	Joback Method
cpg	572.48	J/mol×K	1072.05	Joback Method
cpg	550.47	J/mol×K	986.56	Joback Method
dvisc	0.0000094	Pa×s	608.50	Joback Method
dvisc	0.0000005	Pa×s	815.59	Joback Method
dvisc	0.0000007	Pa×s	781.08	Joback Method
dvisc	0.0000011	Pa×s	746.56	Joback Method
dvisc	0.0000017	Pa×s	712.05	Joback Method
dvisc	0.0000029	Pa×s	677.53	Joback Method
dvisc	0.0000051	Pa×s	643.01	Joback Method
hfust	35.60	kJ/mol	436.80	NIST Webbook
hfust	22.00	kJ/mol	343.00	NIST Webbook
hsubt	228.00	kJ/mol	322.50	NIST Webbook
hvapt	75.60	kJ/mol	411.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	445.70	K	0.10	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=C131533&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume