1-Propanone, 2-hydroxy-1-[4-(2-hydroxyethoxy)phenyl]-2-methy

Other names: 1-[4-(2-Hydroxyethoxy)phenyl]-2-hydroxy-2-methyl-1-propan-1-one
1-[4-(2-Hydroxyethoxy)phenyl]-2-hydroxy-2-methyl-1-propanone
2-Hydroxy-1-[4-(2-hydroxyethoxy)phenyl]-2-methyl-1-propanone
2-Hydroxy-4'-(2-hydroxyethoxy)-2-methylpropiophenone
4-(2-Hydroxyethoxy)phenyl 2-hydroxy-2-propyl ketone
D 2959
DC 2959
Darocur 2595
Darocur 2959
I 2959
IRG 2959
IRGC 2959
Irgacure 2959
UV 2959
ZLI 2959
2-hydroxy-4-hydroxyethoxy-2-methylpropiophenone
Irgacure 2959 (2-Hydroxy-1-[4-(2-hydroxyethoxy) phenyl]-2-methyl-1-propanone)

Inchi: InChI=1S/C12H16O4/c1-12(2,15)11(14)9-3-5-10(6-4-9)16-8-7-13/h3-6,13,15H,7-8H2,1-2

InchiKey: GJKGAPPUXSSCFI-UHFFFAOYSA-N

Formula: C12H16O4

SMILES: CC(C)(O)C(=O)c1ccc(OCCO)cc1

Mol. weight [g/mol]: 224.25

CAS: 106797-53-9

Physical Properties

Property code	Value	Unit	Source
gf	-351.78	kJ/mol	Joback Method
hf	-623.96	kJ/mol	Joback Method
hfus	24.04	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.011		Crippen Method
mcvol	175.360	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
rinpol	1914.00		NIST Webbook
tb	763.04	K	Joback Method
tc	959.00	K	Joback Method

tf	460.16	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.57	J/mol×K	763.04	Joback Method
cpg	512.84	J/mol×K	795.70	Joback Method
cpg	522.44	J/mol×K	828.36	Joback Method
cpg	531.40	J/mol×K	861.02	Joback Method
cpg	539.76	J/mol×K	893.68	Joback Method
cpg	547.54	J/mol×K	926.34	Joback Method
cpg	554.79	J/mol×K	959.00	Joback Method
dvisc	0.0007004	Pa×s	460.16	Joback Method
dvisc	0.0002162	Pa×s	510.64	Joback Method
dvisc	0.0000825	Pa×s	561.12	Joback Method
dvisc	0.0000369	Pa×s	611.60	Joback Method
dvisc	0.0000187	Pa×s	662.08	Joback Method
dvisc	0.0000104	Pa×s	712.56	Joback Method
dvisc	0.0000063	Pa×s	763.04	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C106797539&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume